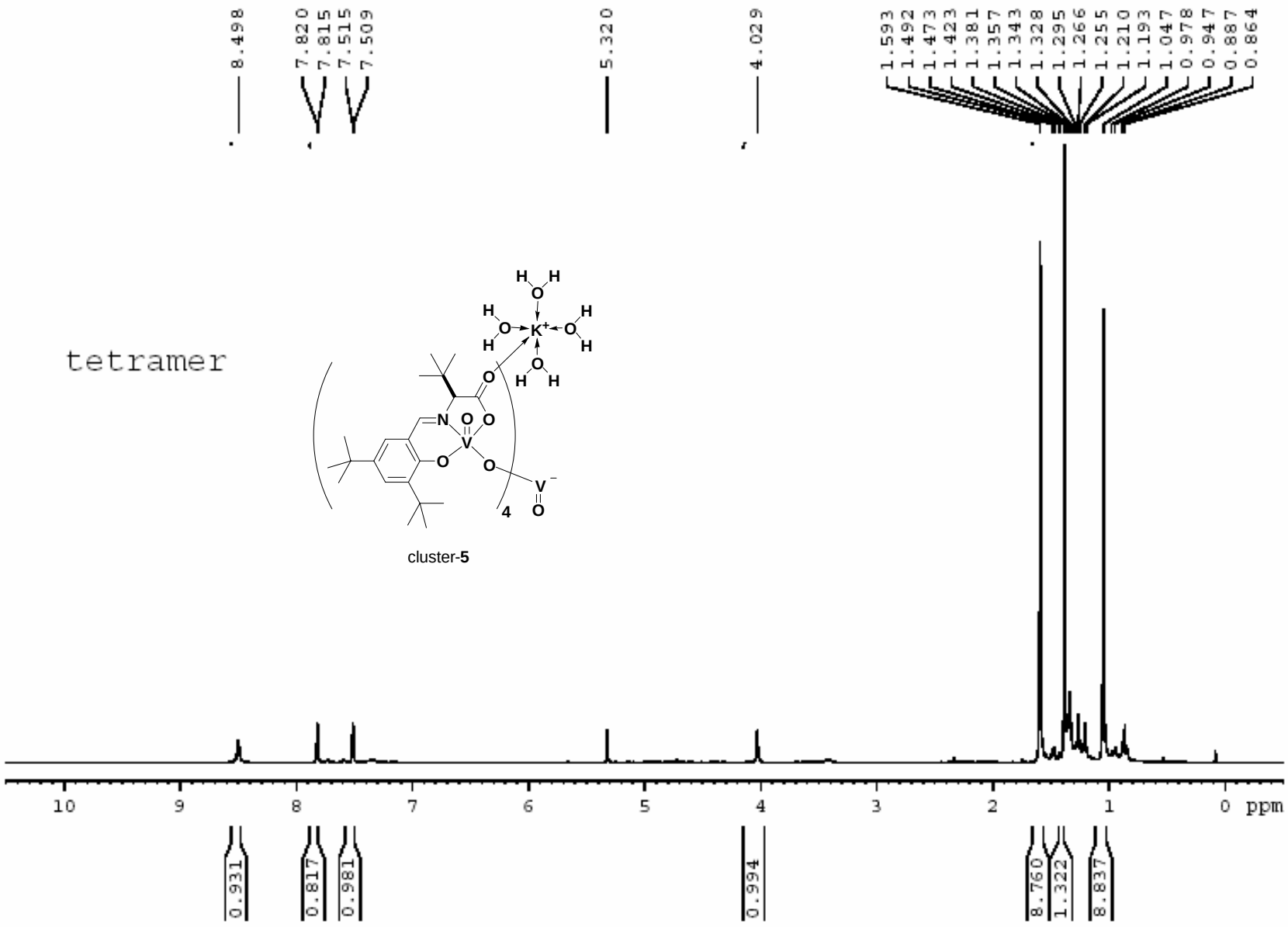
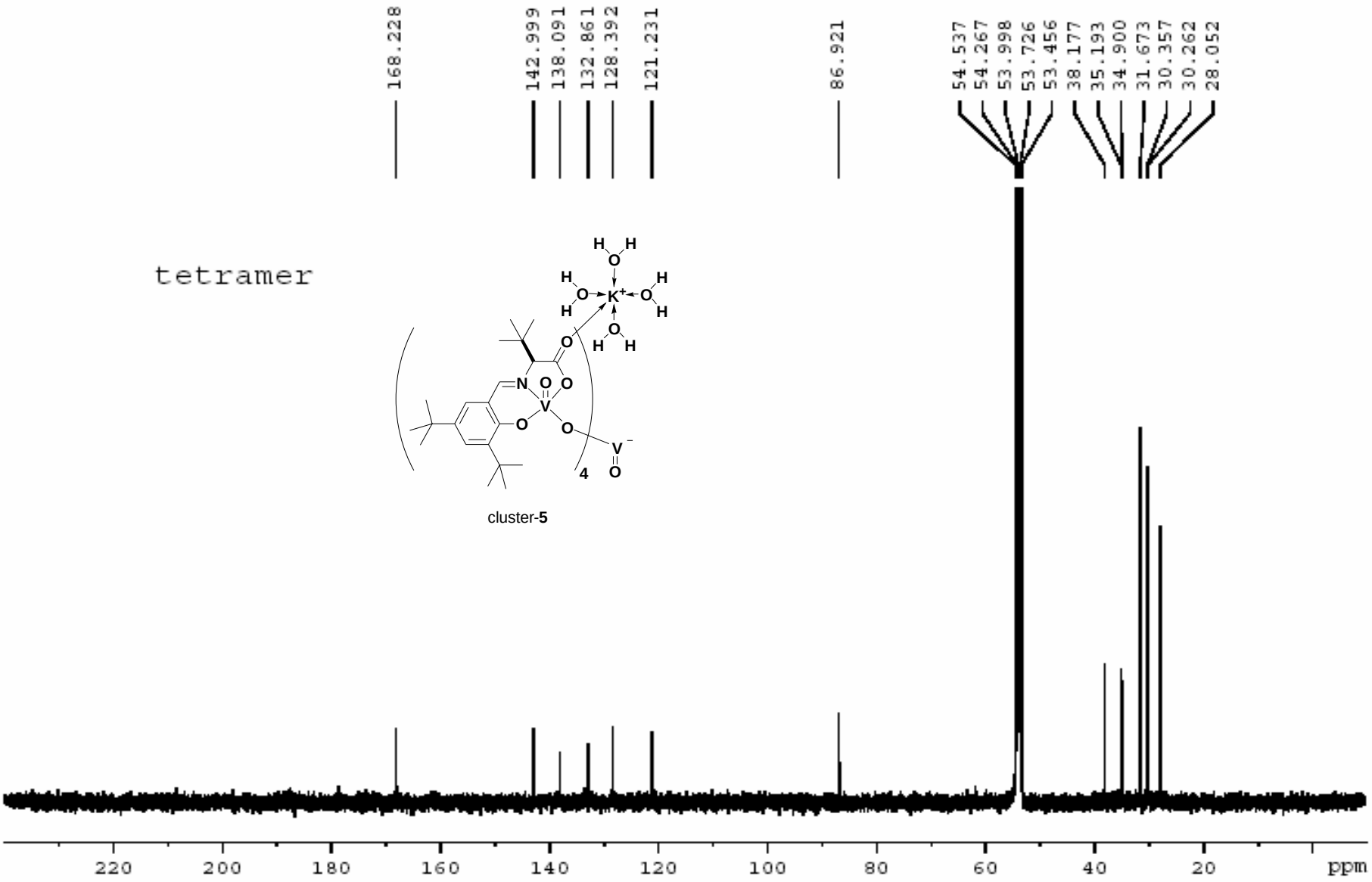
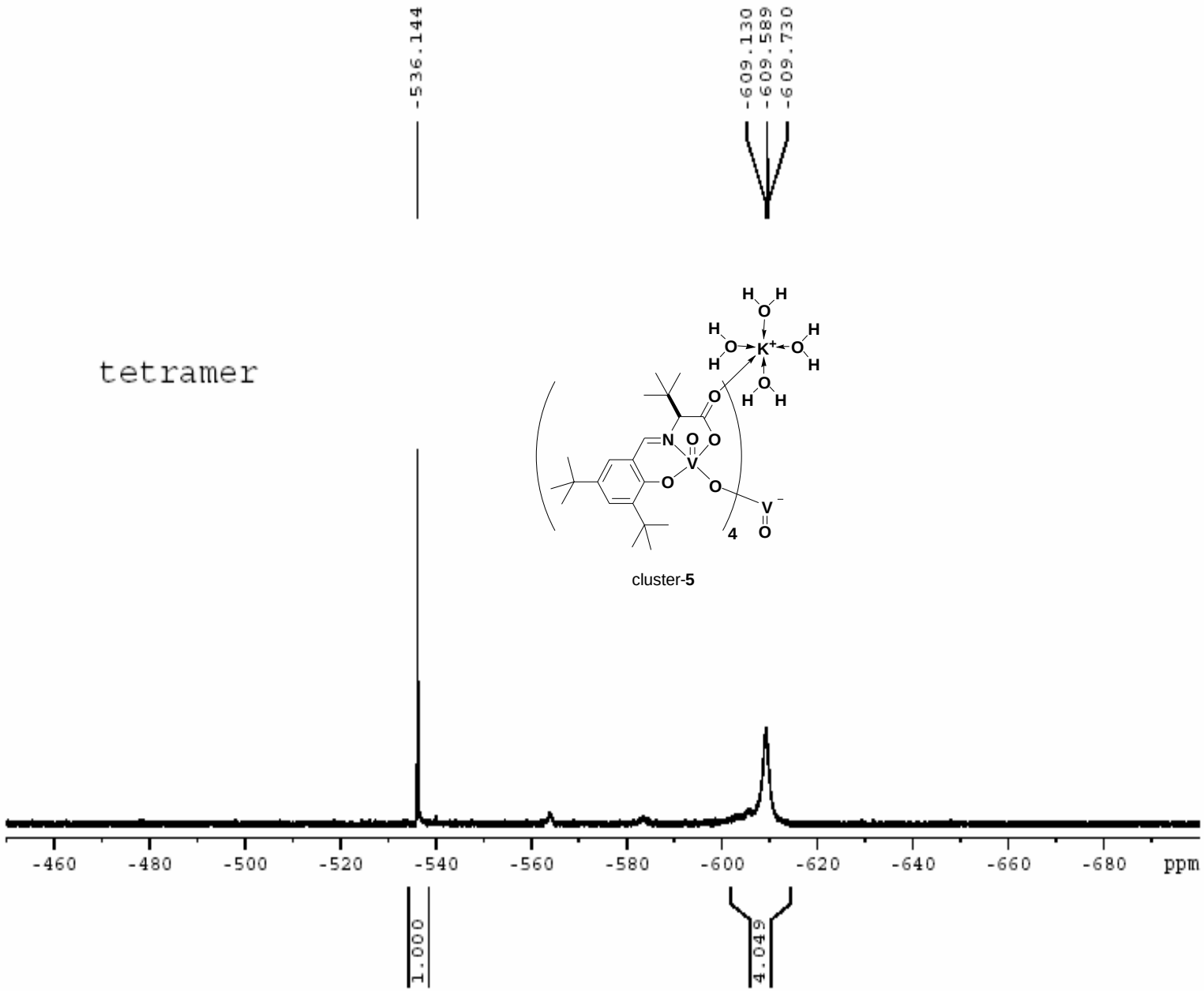
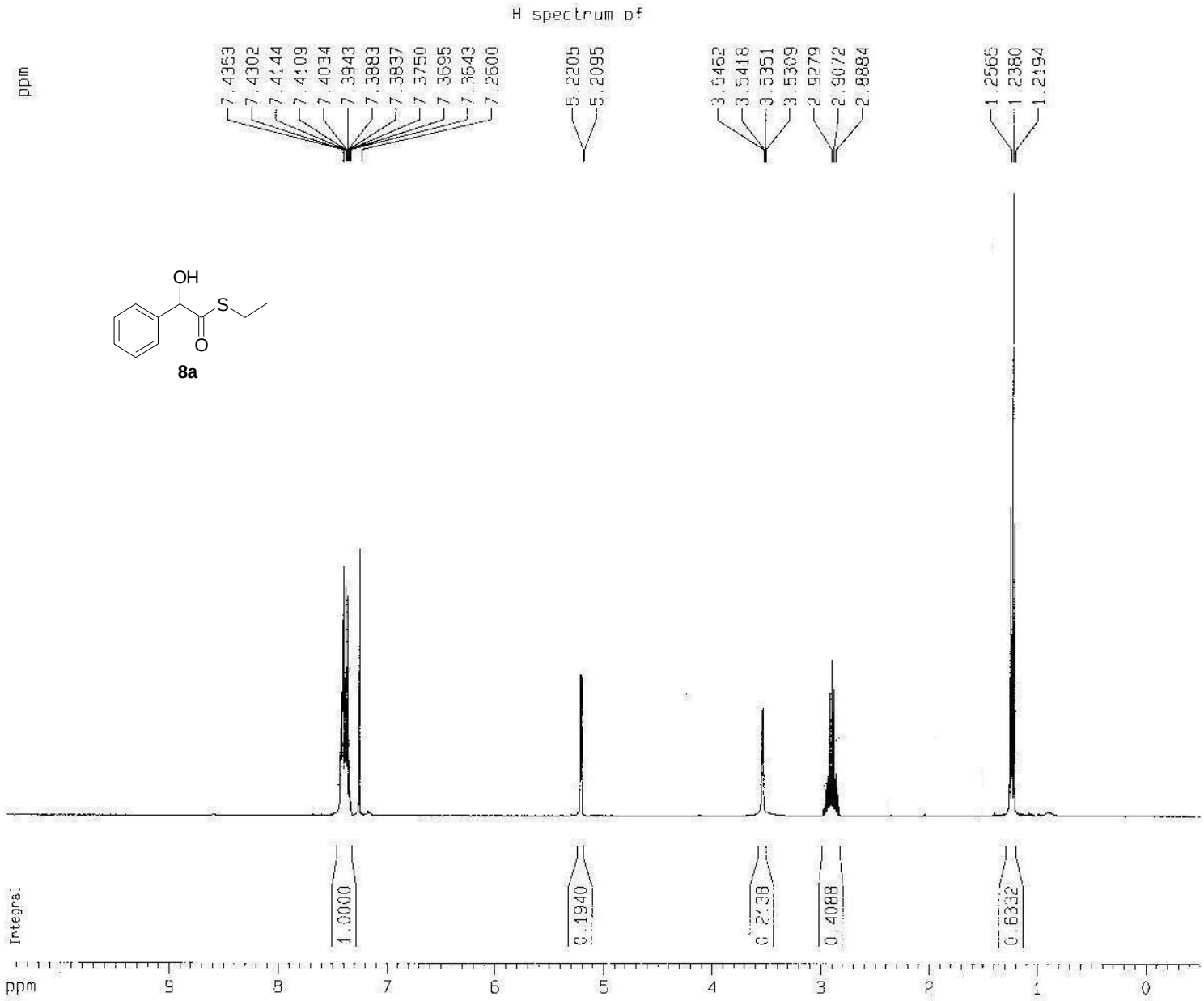
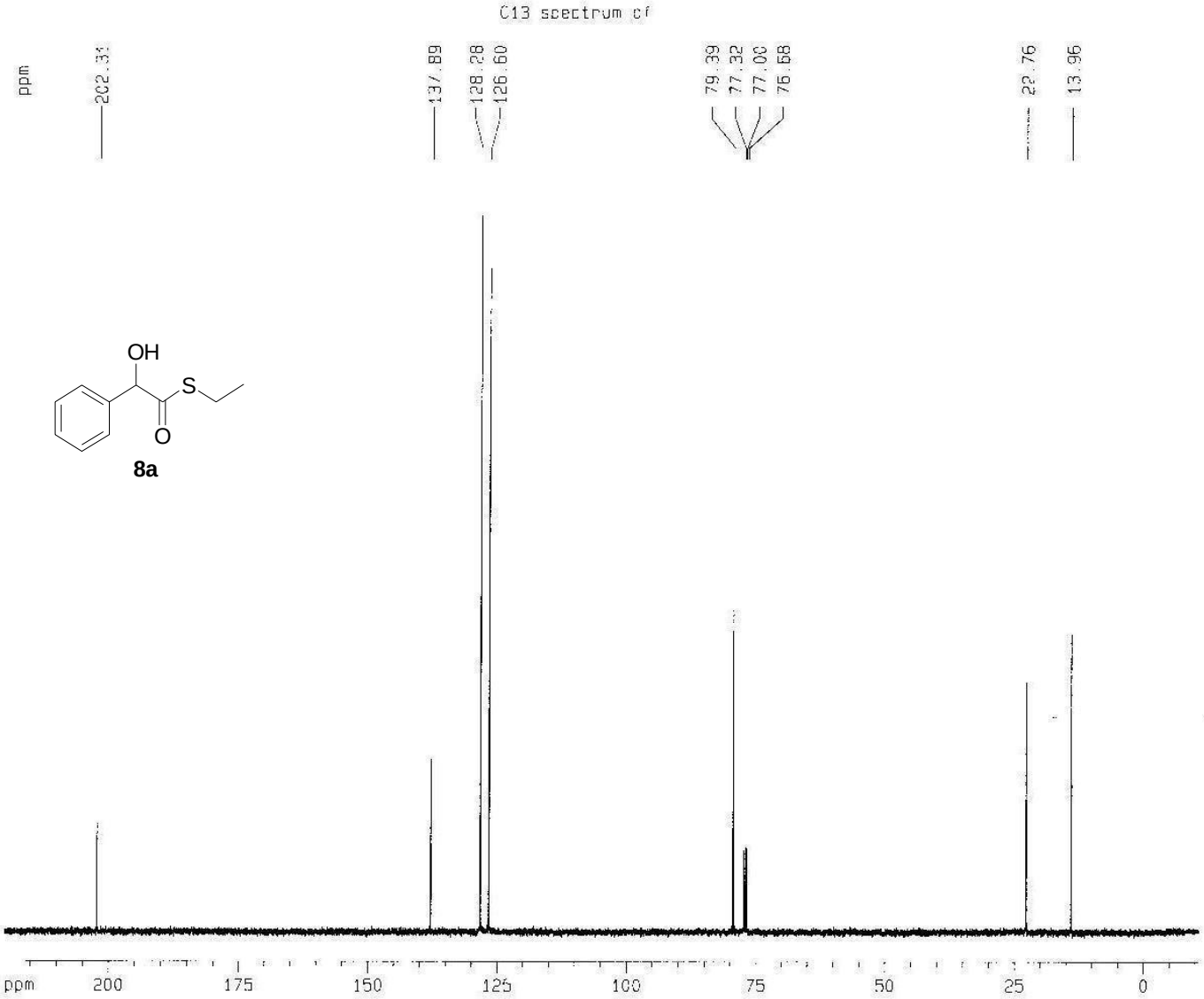

8.498
7.820
7.815
7.515
7.509
5.320
4.029
1.593
1.492
1.473
1.423
1.381
1.357
1.343
1.328
1.295
1.266
1.255
1.210
1.193
1.047
0.978
0.947
0.887
0.864
tetramer
cluster-5
10
9
8
7
6
5
4
3
2
1
0 ppm
0.931
0.817
0.981
0.994
8.760
1.322
8.837


168.228
142.999
138.091
132.861
128.392
121.231
86.921
54.537
54.267
53.998
53.726
53.456
38.177
35.193
34.900
31.673
30.357
30.262
28.052
tetramer
cluster-5
220
200
180
160
140
120
100
80
60
40
20
ppm

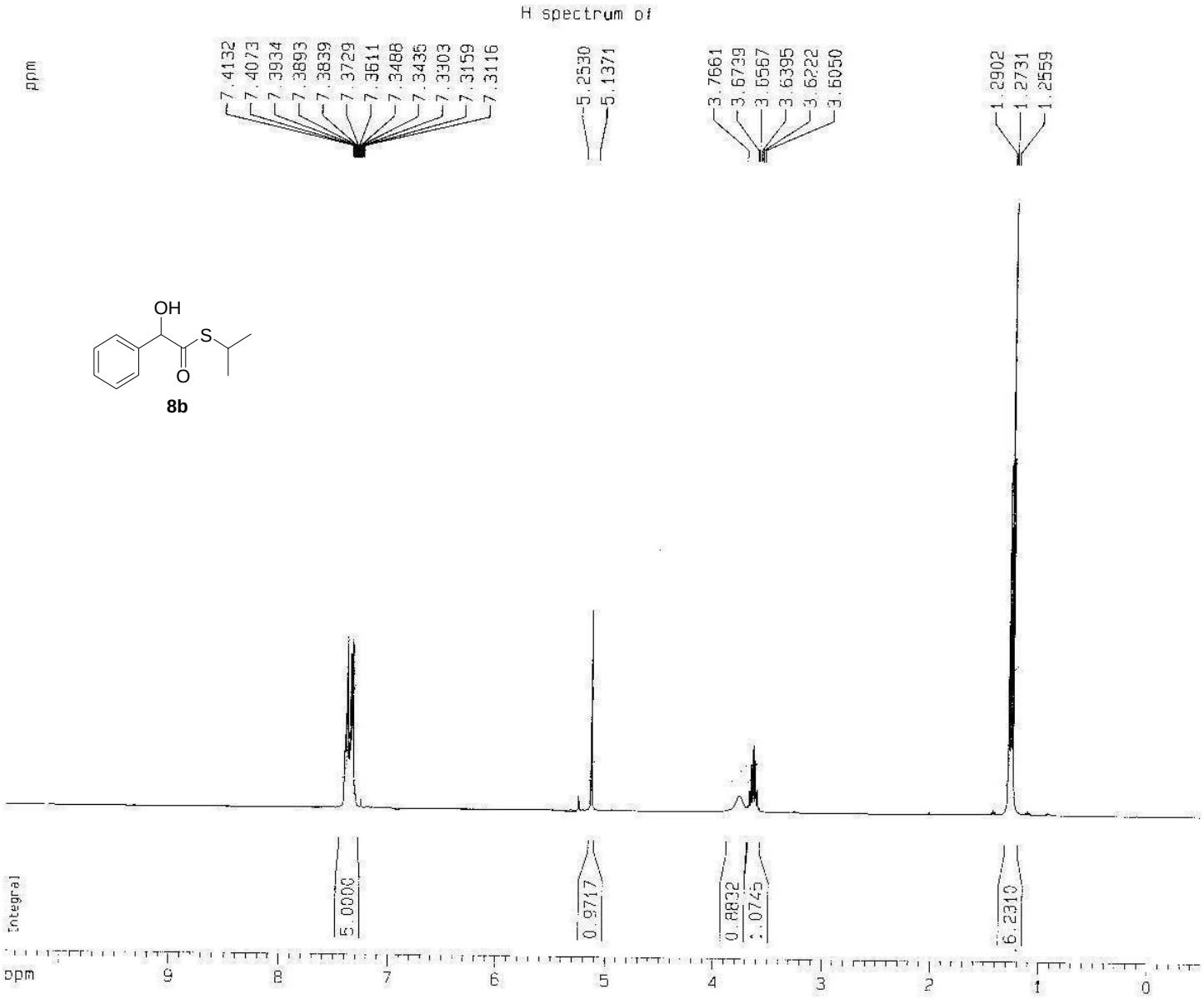

-536.144
-609.130
-609.589
-609.730
tetramer
cluster-5
-460
-480
-500
-520
-540
-560
-580
-600
-620
-640
-660
-680
ppm
1.000
4.049



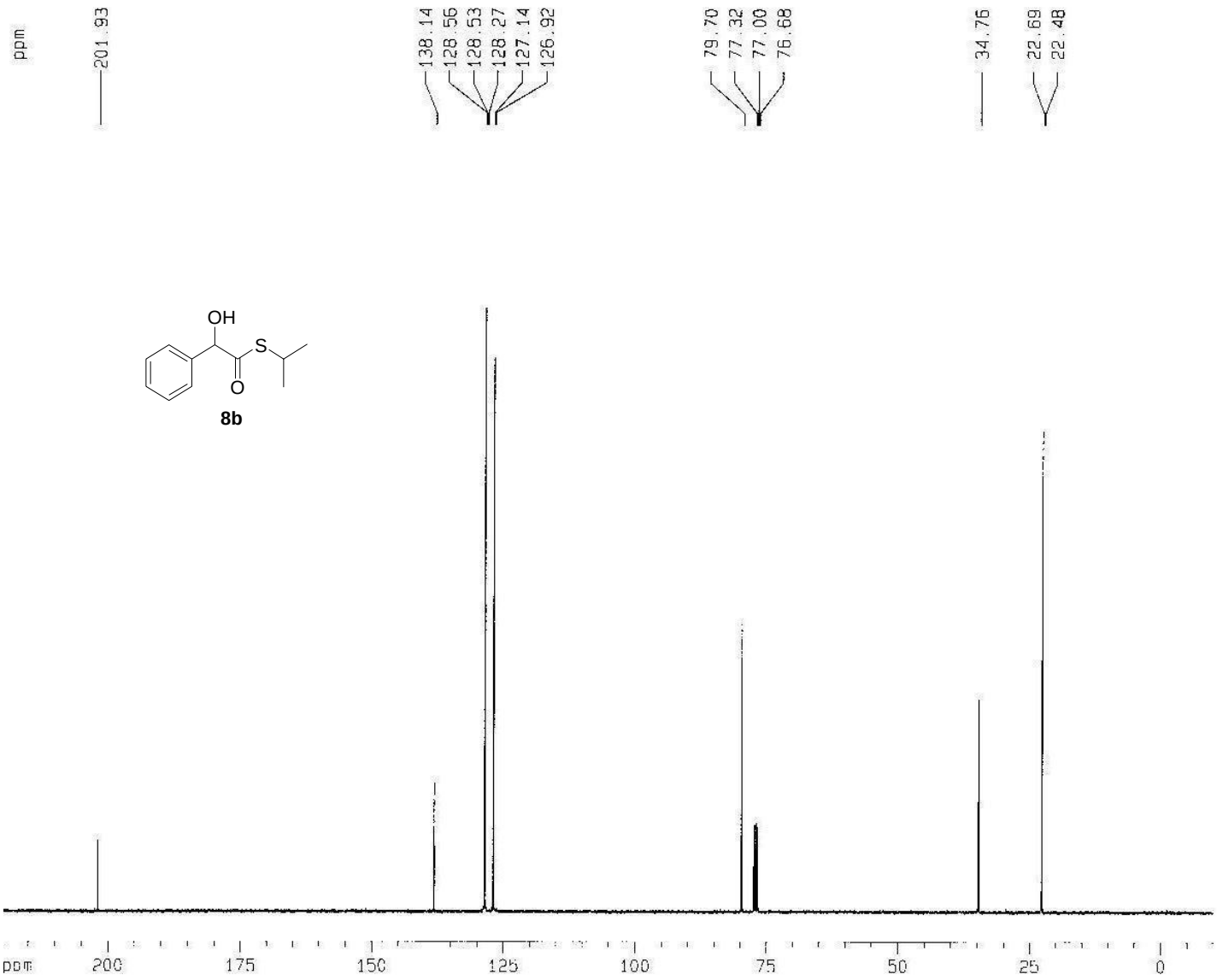

```
NAME        eth thio est
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20051021
Time              20 37
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                16384
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            5995.204 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                  362
DW               83.400 usec
DE                6.50 usec
TE               300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.10 usec
PL1                3.00 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300095 MHz
WDW                  EM
SSB                   0
LB                 0.10 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                10.50 cm
F1P              10.500 ppm
F1              4201.37 Hz
F2P              -0.500 ppm
F2              -200.07 Hz
PPMCM           0.55000 ppm/cm
HZCM          220.07152 Hz/cm
```



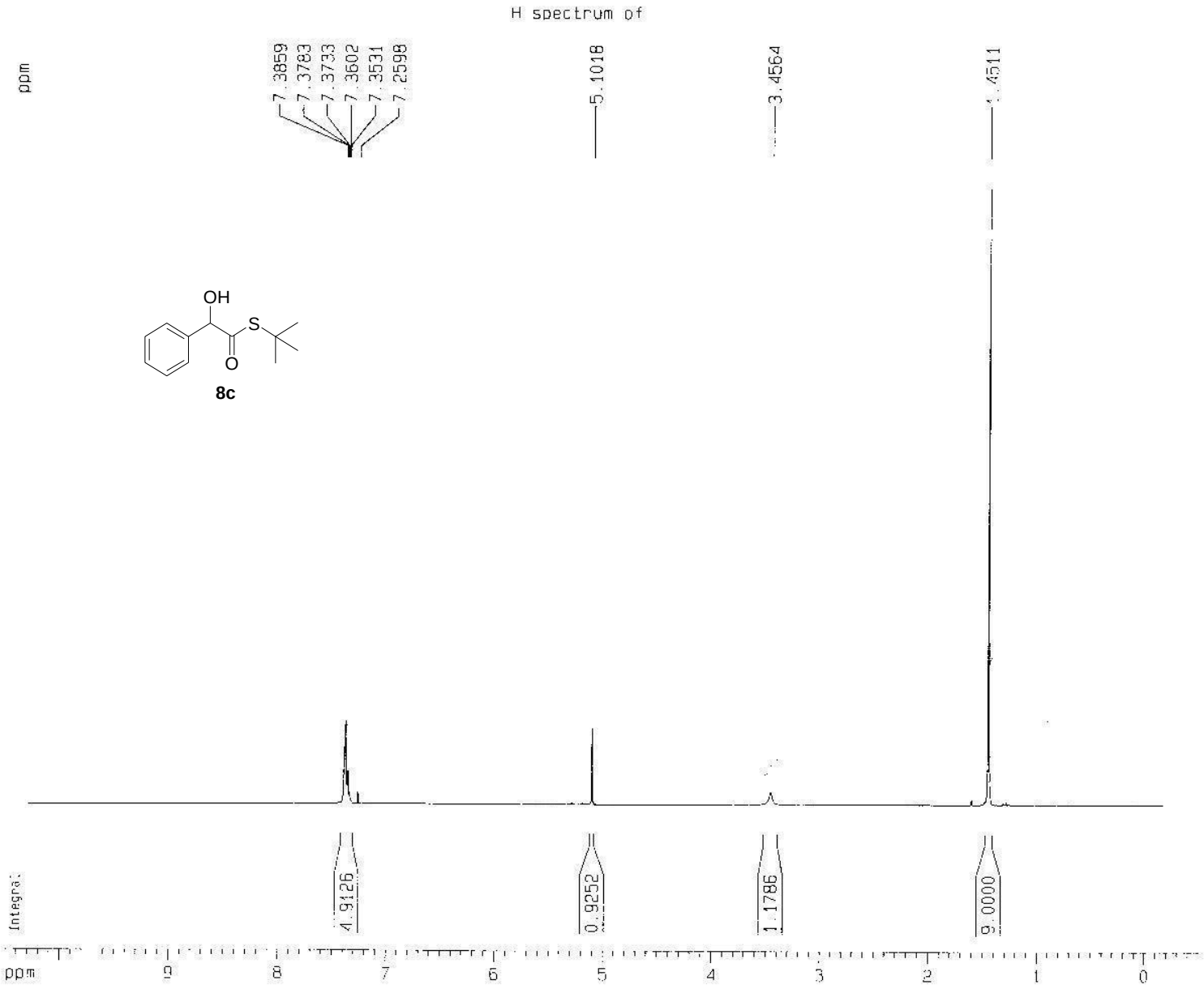

```
Current Data Parameters
NAME          ethane thio
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20051027
Time               14.50
INSTRUM            spect
PROBHD   5 mm BBO BB 1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                    9
DS                    0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ            1.3042164 sec
RG                 8192
DW               19.900 usec
DE                6.50 usec
TE                300.0 K
D1            1.20000005 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.80 usec
PL1                 7.00 dB
SFO1         100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 3.00 dB
PL12               21.83 dB
PL13               24.80 dB
SFO2         400.1319000 MHz

F2 - Processing parameters
SI                 32768
SF           100.6128120 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 12.50 cm
F1P               220.000 ppm
F1              22134.82 Hz
F2P                10.688 ppm
F2              -1075.30 Hz
PPMCM           11.53438 ppm/cm
HZCM          1160.50623 Hz/cm
```



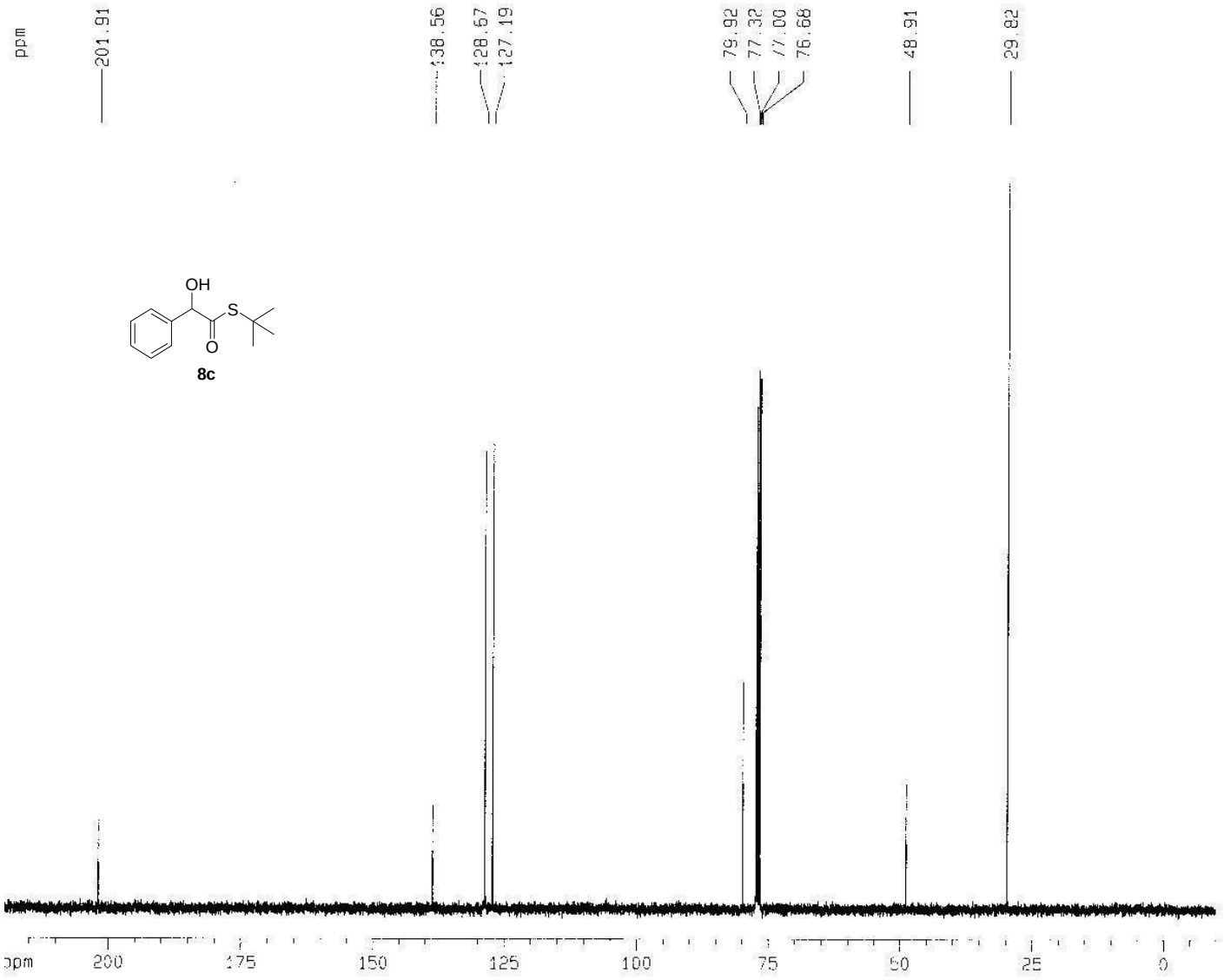

```
NAME          sam-iso HT1
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20060528
Time               16.07
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                16384
SOLVENT           CDCl3
NS                   16
DS                    0
SWH           5995.204 Hz
FIDRES        0.365918 Hz
AQ          1.3664756 sec
RG                 22.6
DW               83.400 usec
DE                6.50 usec
TE               300.0 K
D1          1.50000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1               10.10 usec
PL1               3.00 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                16384
SF        400.1300088 MHz
WDW                  EM
SSB                   0
LB                 0.10 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                10.50 cm
F1P               10.500 ppm
F1              4201.37 Hz
F2P               -0.500 ppm
F2              -200.07 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07152 Hz/cm
```



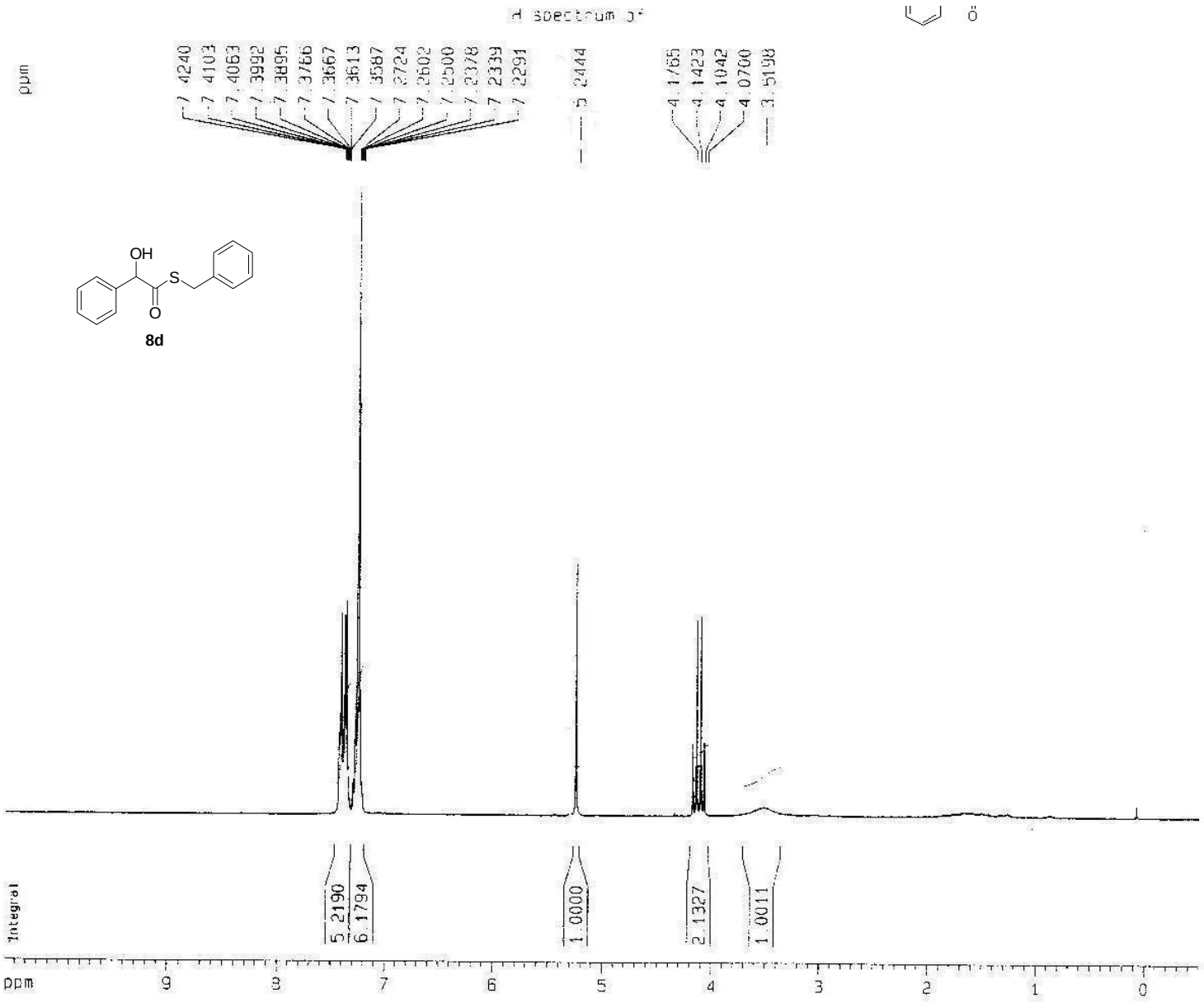

```
Current Data Parameters
NAME          sam-150 HT1
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_            20060528
Time               16.14
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  174
DS                    0
SWH            25125.629 Hz
FIDRES          0.383387 Hz
AQ             1.3042164 sec
RG                 8192
DW                19.900 usec
DE                 6.50 usec
TE                300.0 K
D1            1.20000005 sec
D11           0.03000000 sec
D12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                10.80 usec
PL1                7.00 dB
SFO1         100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.80 dB
SFO2         400.1319000 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127874 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 10.00 cm
F1P               220.000 ppm
F1                22134.81 Hz
F2P               -10.000 ppm
F2                -1006.13 Hz
PPMCM             11.50000 ppm/cm
HZCM           1157.04700 Hz/cm
```



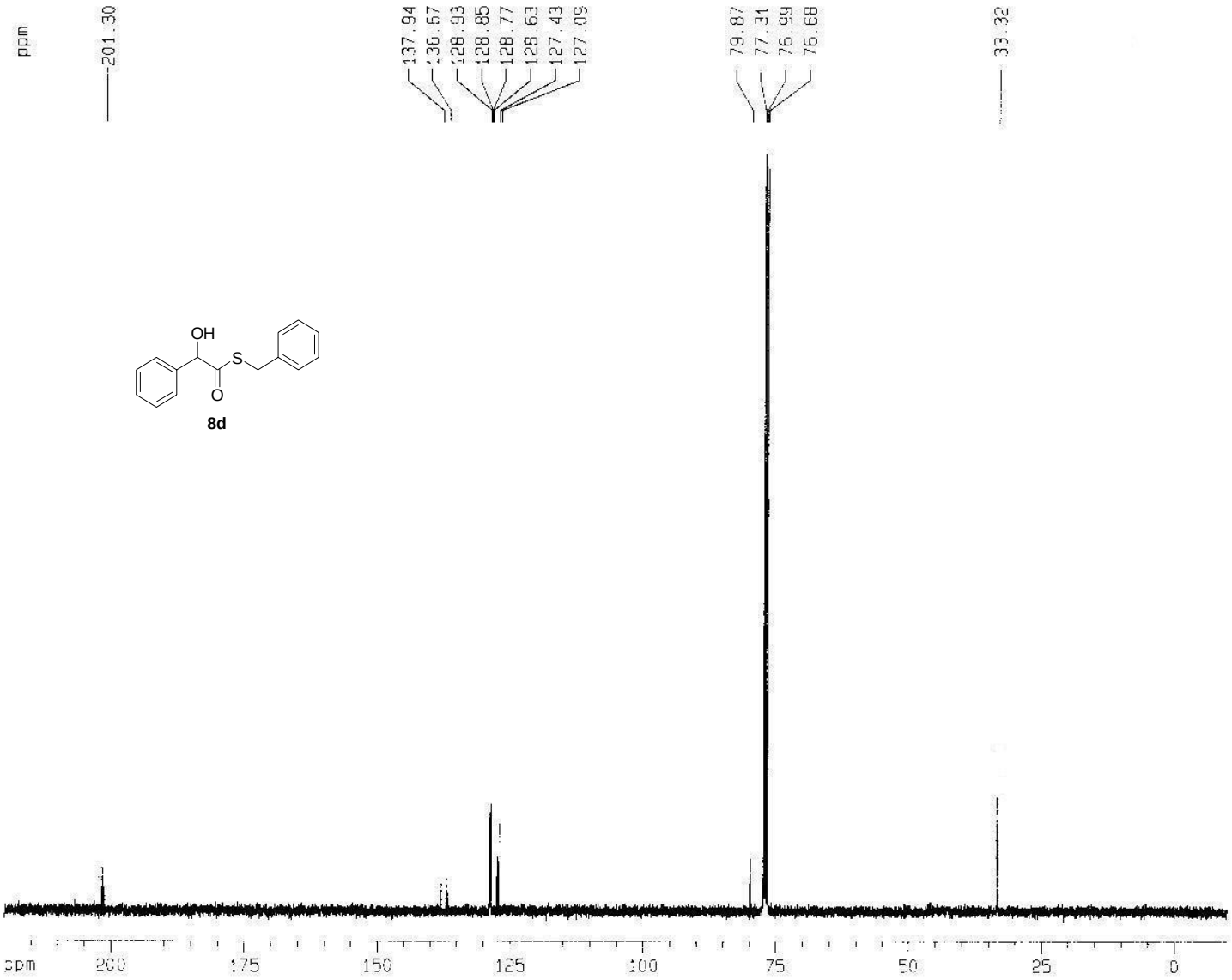

```
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20060528
Time              14.45
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                16384
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            5995.204 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                101.6
DW               83.400 usec
DE                6.50 usec
TE                300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.10 usec
PL1               3.00 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300091 MHz
WDW                  EM
SSB                   0
LB                 0.10 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                10.50 cm
F1P               10.500 ppm
F1              4201.37 Hz
F2P               -0.500 ppm
F2              -200.07 Hz
PPMCM           0.55000 ppm/cm
HZCM          220.07152 Hz/cm
```



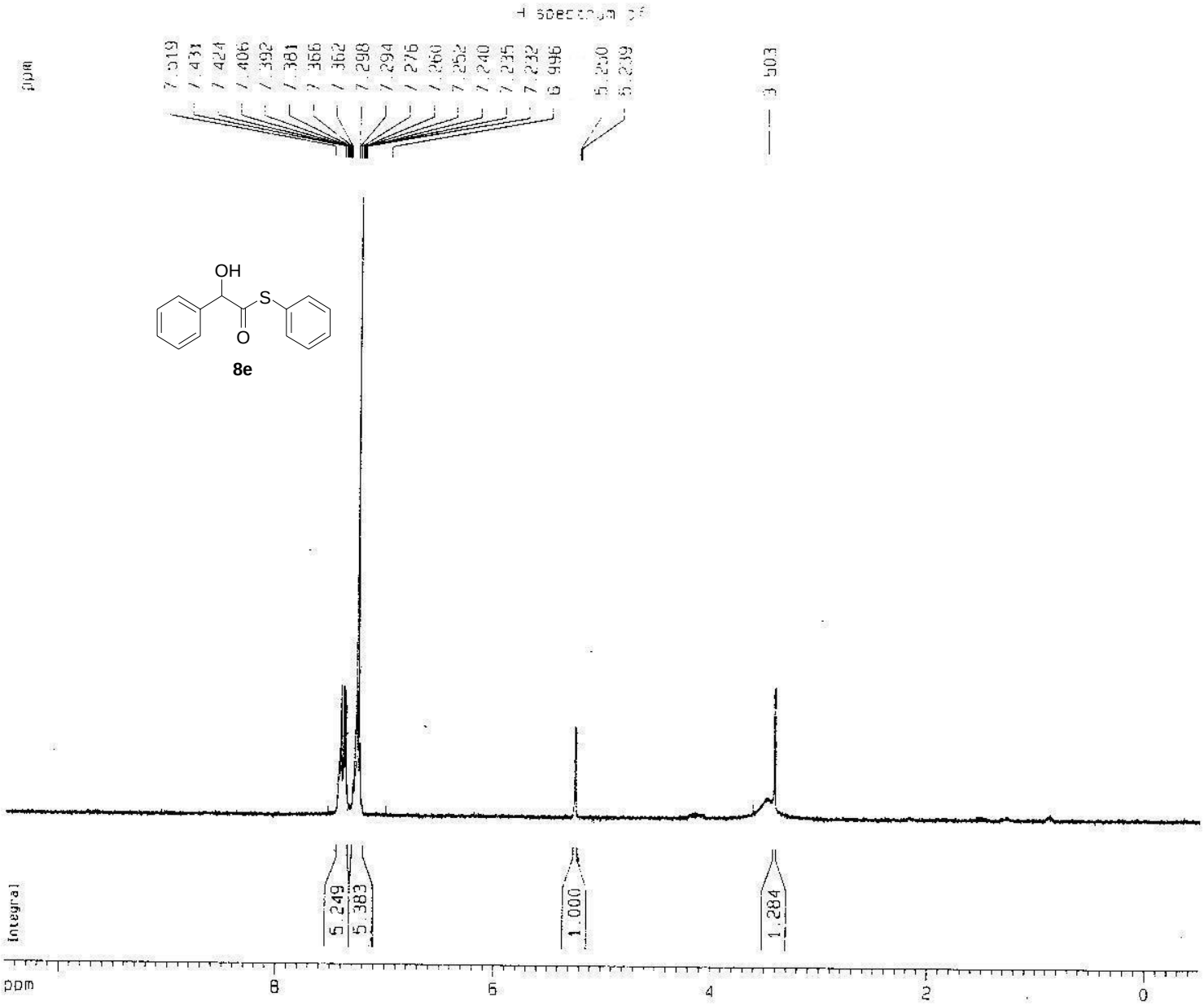

```
Current Data Parameters
NAME      saw-phen HT-h2
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_          20080529
Time               14.48
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  180
DS                    0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ            1.3042164 sec
RG                 4096
DW               19.900 usec
DE                6.50 usec
TE               300.0 K
D1            1.20000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.80 usec
PL1                7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127736 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 12.50 cm
F1P             220.000 ppm
F1              22134.81 Hz
F2P              -10.000 ppm
F2              -1006.13 Hz
PHMCM           11.50000 ppm/cm
HZCM          1157.04868 Hz/cm
```



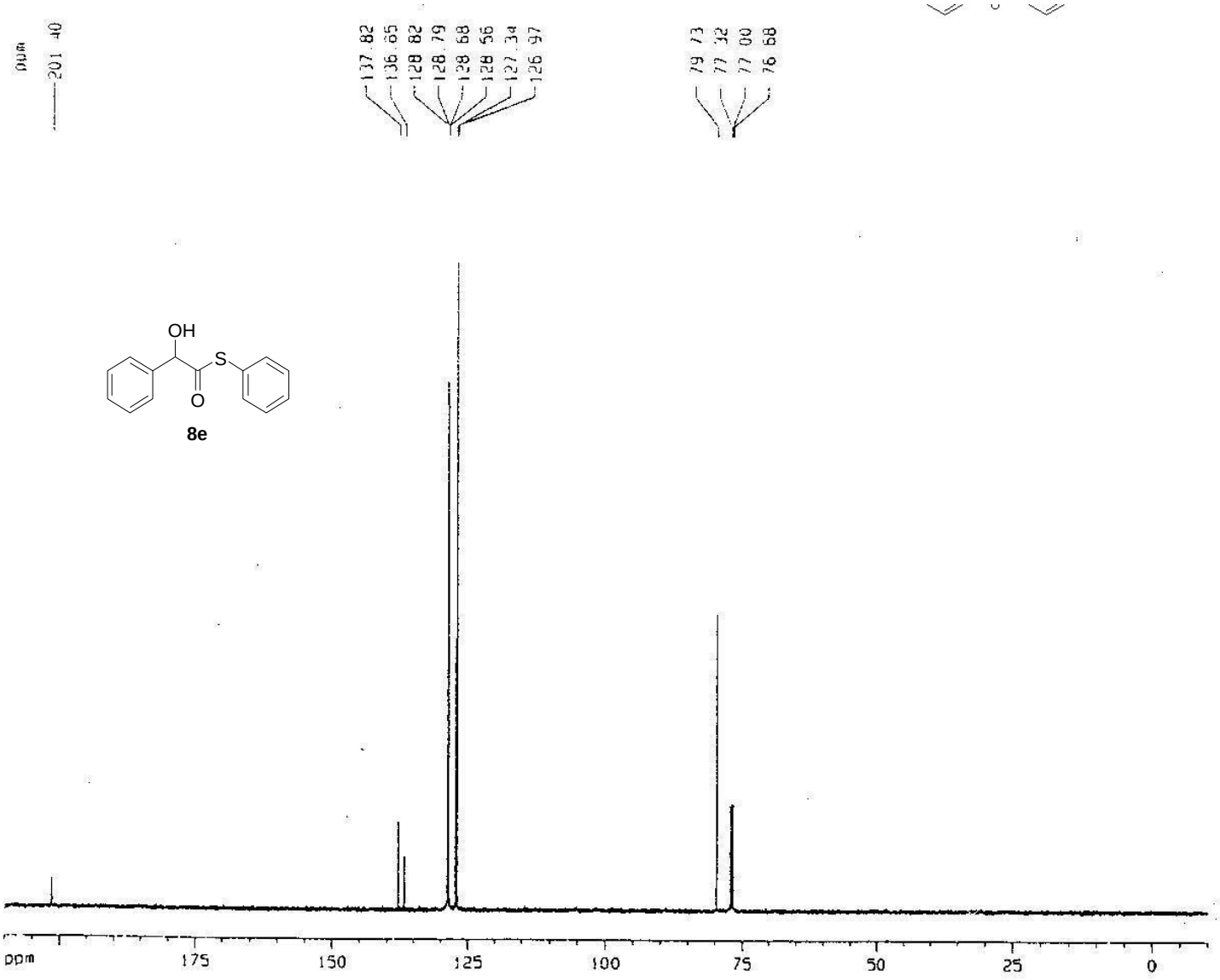

```
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20060528
Time              15.04
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG           zg30
TD                16384
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            6995.204 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                 322.5
DW               83.400 usec
DE                6.50 usec
TE               300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.10 usec
PL1                3.00 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300091 MHz
WDW                  EM
SSB                   0
LB                 0.10 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                10.50 cm
F1P               10.500 ppm
F1                4201.37 Hz
F2P               -0.500 ppm
F2                -200.07 Hz
PPMCM             0.55000 ppm/cm
HZCM            220.07152 Hz/cm
```



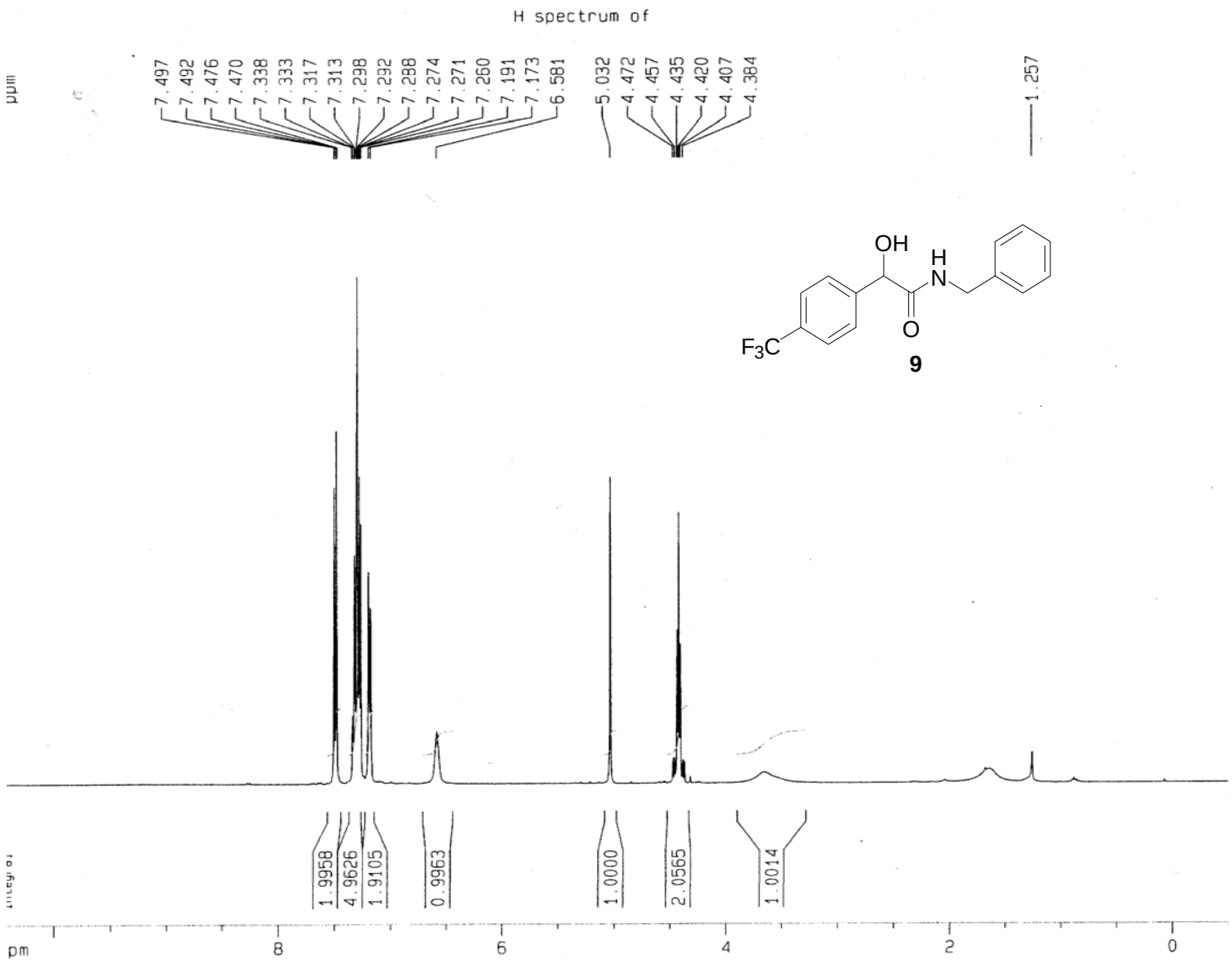

```
Current Data Parameters
NAME      sam-5 Benzyl-HI-H1
EXPNO                     4
PROCNO                    1

F2 - Acquisition Parameters
Date_           20050528
Time                 15.10
INSTRUM              spect
PROBHD   5 mm BBO 68 1H
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     500
DS                       0
SWH             25125.629 Hz
FIDRES           0.383387 Hz
AQ               1.3042164 sec
RG                    4096
DW                  19.900 usec
DE                   6.50 usec
TE                  300.0 K
D1              1.20000005 sec
d11             0.03000000 sec
d12             0.00002000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                   10.80 usec
PL1                   7.00 dB
SFO1          100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                   3.00 dB
PL12                 21.83 dB
PL13                 24.80 dB
SFO2          400.1319000 MHz

F2 - Processing parameters
SI                   32768
SF            100.6127713 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40

1D NMR plot parameters
CX                   20.00 cm
CY                   12.50 cm
F1P                 220.000 ppm
F1                 22134.81 Hz
F2P                 -10.000 ppm
F2                -1006.13 Hz
PPMCM              11.00000 ppm/cm
HZCM            1157.04888 Hz/cm
```




```
NAME                20050815
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20050815
Time                   15.18
INSTRUM                spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                     15384
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 6995.204 Hz
FIDRES              0.365918 Hz
AQ                 1.3664756 sec
RG                     645.1
DW                    83.400 usec
DE                     6.50 usec
TE                    300.0 K
D1                 1.30000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                      10.10 usec
PL1                      3.00 dB
SFO1             400.1326008 MHz

F2 - Processing parameters
SI                     16384
SF               400.1300095 MHz
WDW                       EM
SSB                        0
LB                      0.10 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     20.00 cm
CY                     30.00 cm
F1P                   10.500 ppm
F1                   4201.37 Hz
F2P                   -0.500 ppm
F2                   -200.06 Hz
PPMCM                 0.55000 ppm/cm
HZCM                220.07150 Hz/cm
```

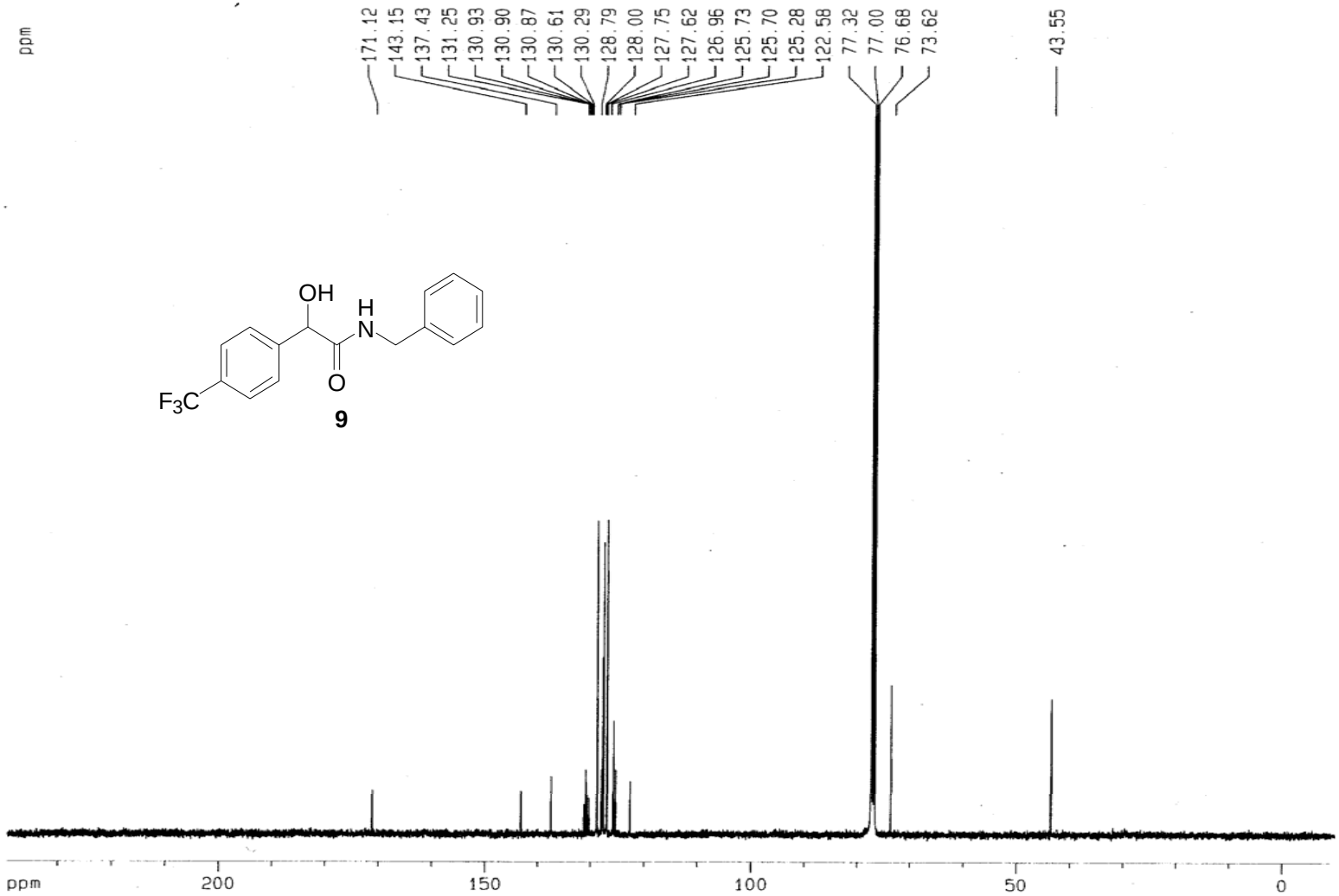



```
Current Data Parameters
NAME      2-exo-06 (C13)
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20060518
Time               15.21
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  183
DS                    0
SWH           25125.629 Hz
FIDRES        0.383387 Hz
AQ            1.3042164 sec
RG                 4096
DW               19.900 usec
DE                6.50 usec
TE               300.0 K
D1            1.20000005 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.80 usec
PL1                7.00 dB
SFO1        100.5242995 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                32768
SF          100.6127844 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                11.00 cm
F1P             210.000 ppm
F1            21128.68 Hz
F2P             -10.000 ppm
F2            -1006.13 Hz
PPMCM           11.00000 ppm/cm
HZCM          1106.74060 Hz/cm
```

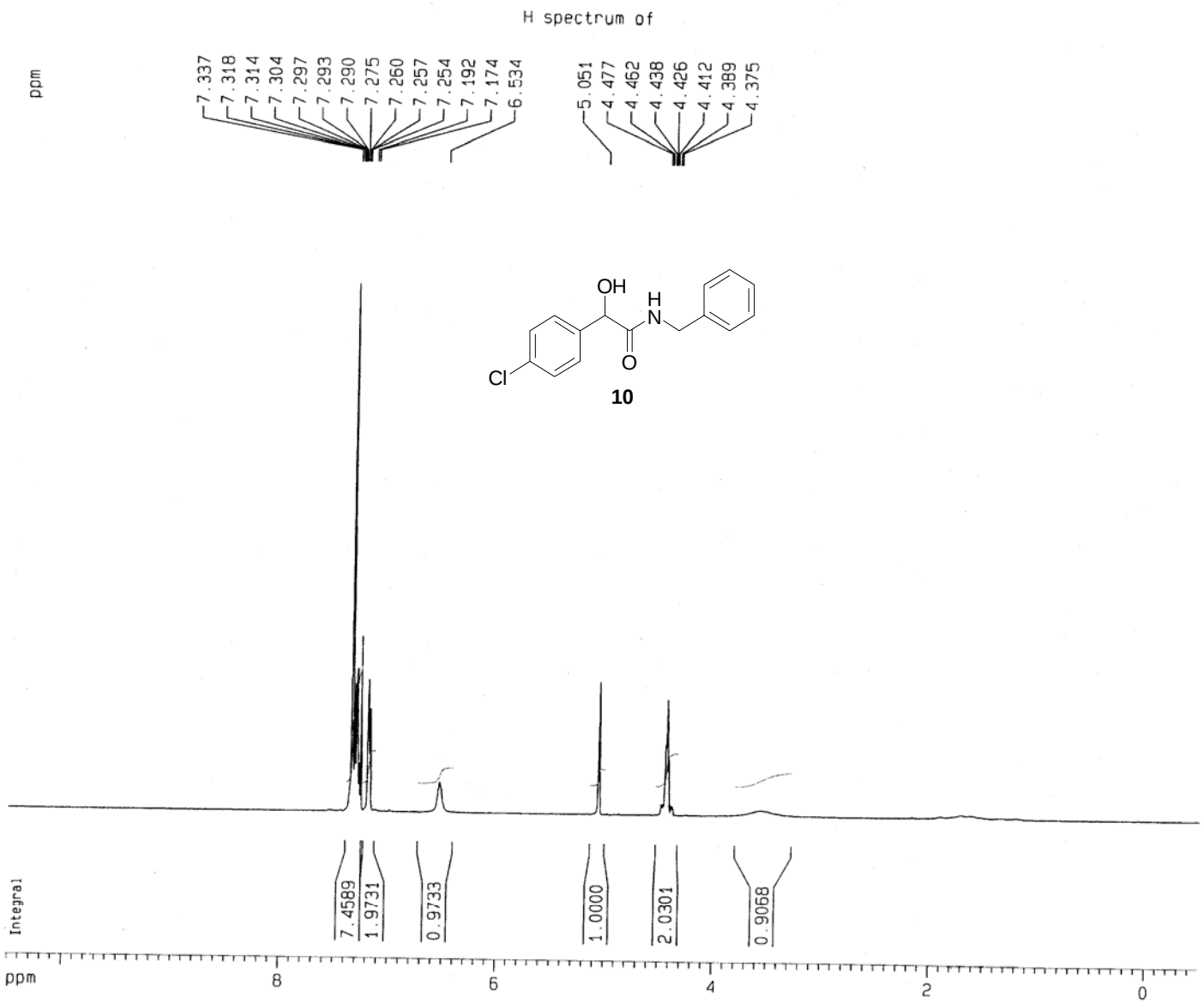



```
NAME          CF3medalate
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20051213
Time               12.41
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                    20
DS                     0
SWH            5995.204 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                 322.5
DW                83.400 usec
DE                 6.50 usec
TE                300.0 K
D1           1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.10 usec
PL1                3.00 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300099 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                  9.00 cm
F1P               10.500 ppm
F1               4201.37 Hz
F2P               -0.500 ppm
F2               -200.07 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07152 Hz/cm
```

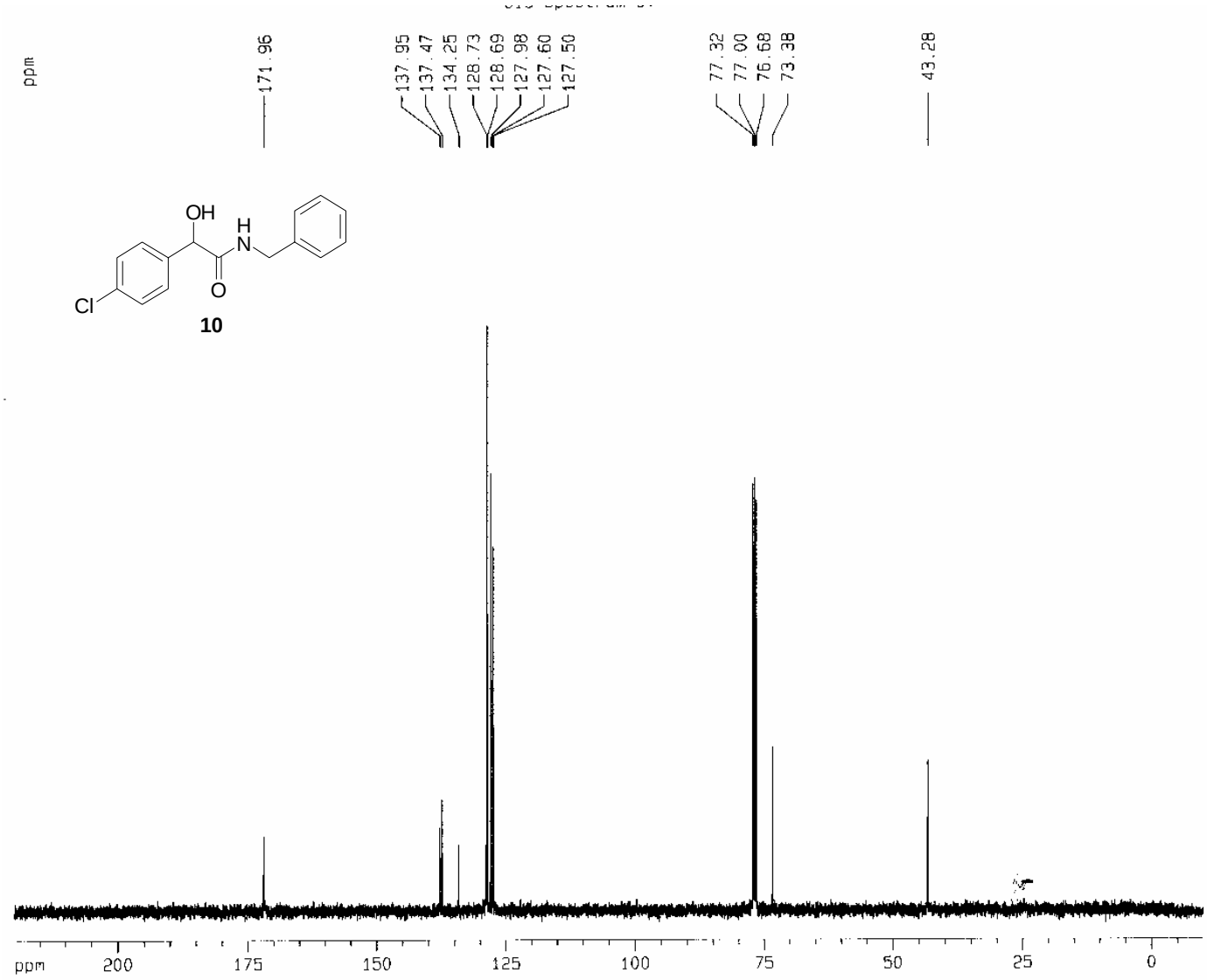
C13 spectrum of



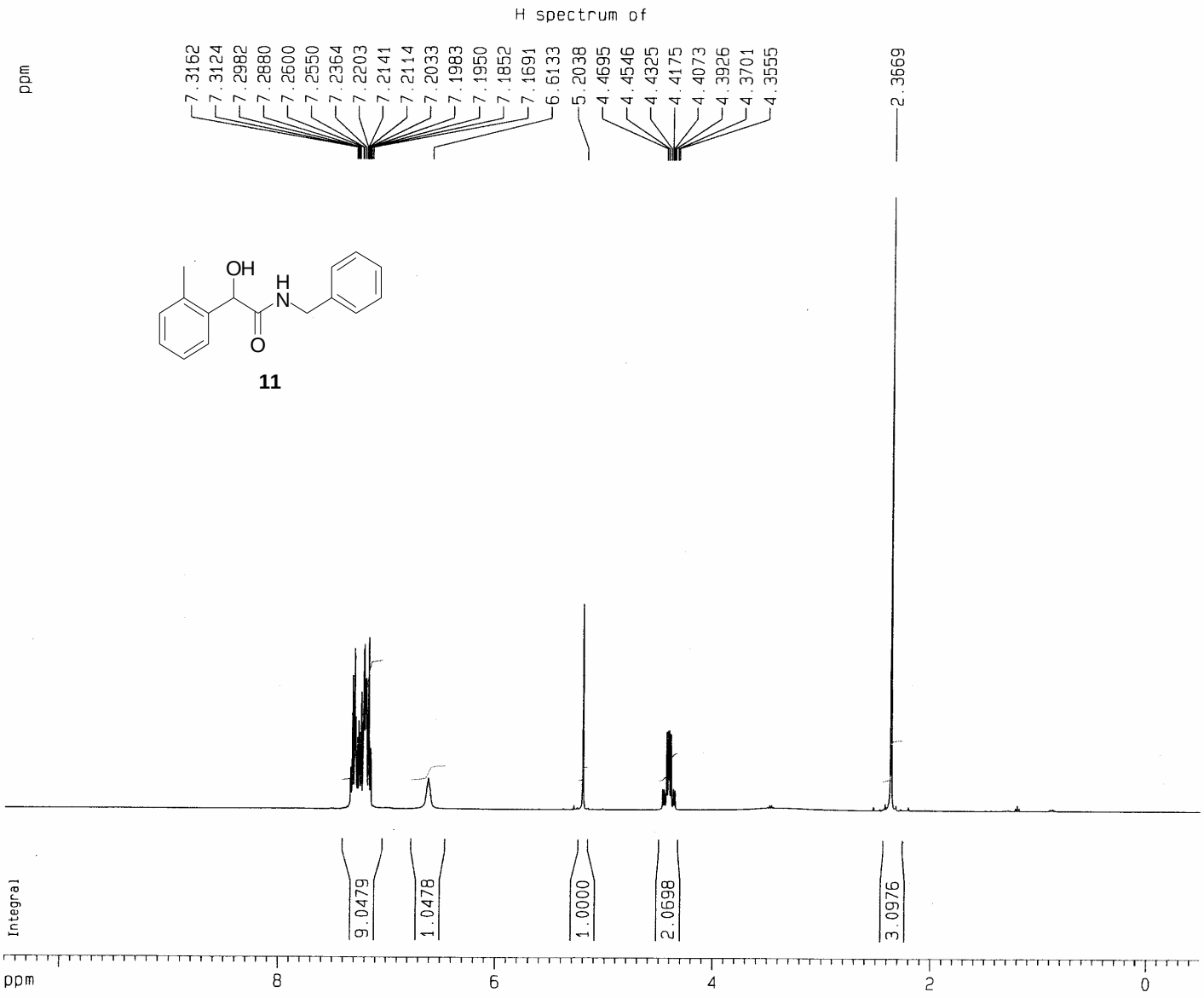

```
Current Data Parameters
NAME      050627.4-CF3-amide
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_            20050630
Time                18.25
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1408
DS                     0
SWH            25125.629 Hz
FIDRES          0.383387 Hz
AQ             1.3042164 sec
RG                  4096
DW                19.900 usec
DE                 6.50 usec
TE                300.0 K
D1            1.20000005 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                10.80 usec
PL1                7.00 dB
SFO1         100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.80 dB
SFO2         400.1319000 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127706 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 30.00 cm
F1P             240.000 ppm
F1             24147.07 Hz
F2P             -10.000 ppm
F2             -1006.13 Hz
PPMCM          12.50000 ppm/cm
HZCM         1257.65967 Hz/cm
```



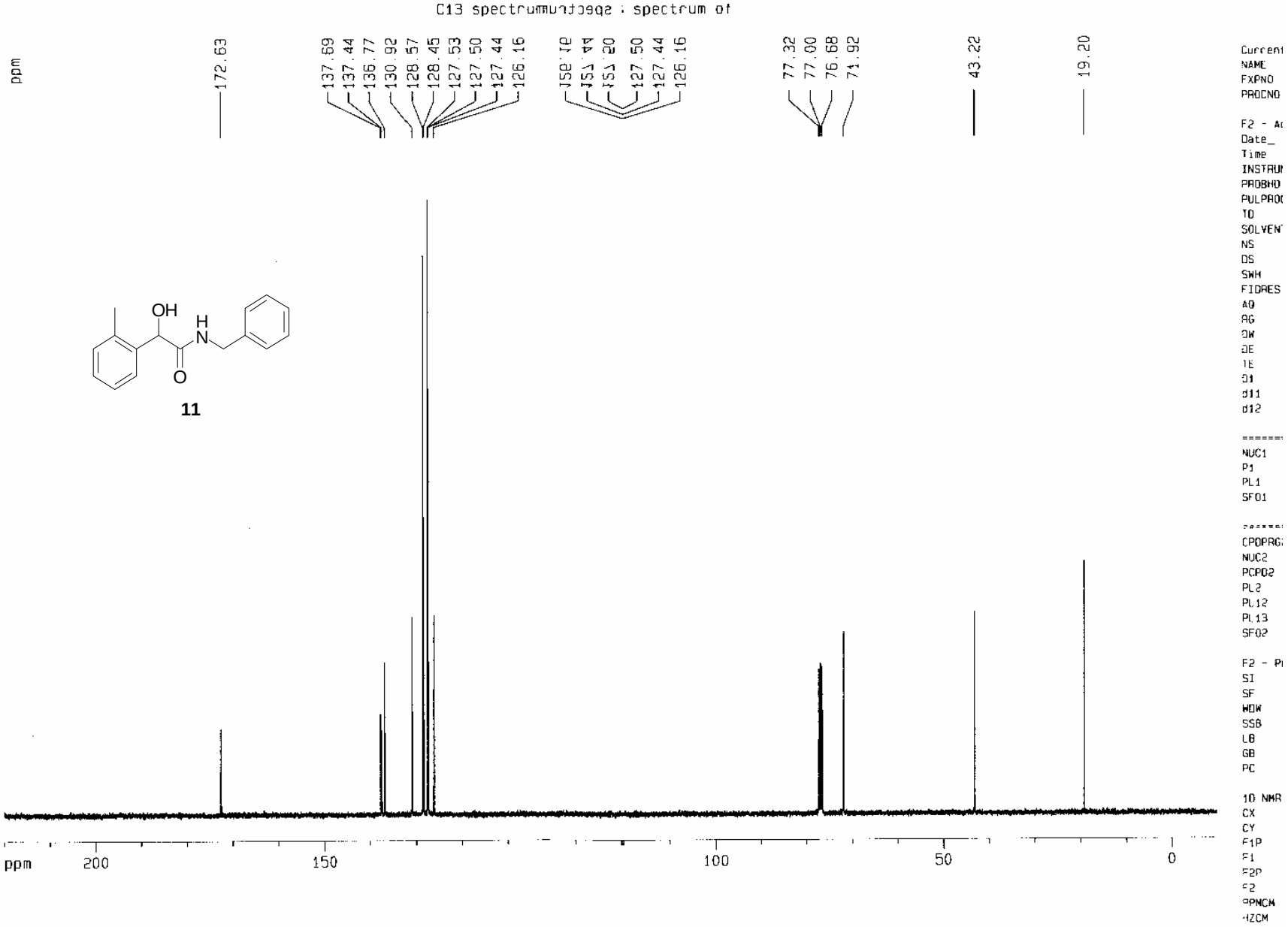

```
Current Data Parameters
NAME        4ClmedelicBnamide
EXPNO                       5
PROCNO                      1

F2 - Acquisition Parameters
Date_               20050319
Time                   19.50
INSTRUM                spect
PROBHD     5 mm BBO BB-1H
PULPROG                 zg30
TD                     16384
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 5995.204 Hz
FIDRES              0.365918 Hz
AQ                 1.3664756 sec
RG                       362
DW                    83.400 usec
DE                     6.50 usec
TE                    300.0 K
D1                 1.50000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                     10.10 usec
PL1                     3.00 dB
SFO1             400.1326008 MHz

F2 - Processing parameters
SI                     16384
SF               400.1300102 MHz
WDW                        EM
SSB                         0
LB                      0.10 Hz
GB                          0
PC                       1.00

1D NMR plot parameters
CX                     20.00 cm
CY                      9.00 cm
F1P                    10.500 ppm
F1                    4201.37 Hz
F2P                    -0.500 ppm
F2                    -200.06 Hz
PPMCM                0.55000 ppm/cm
HZCM               220.07150 Hz/cm
```

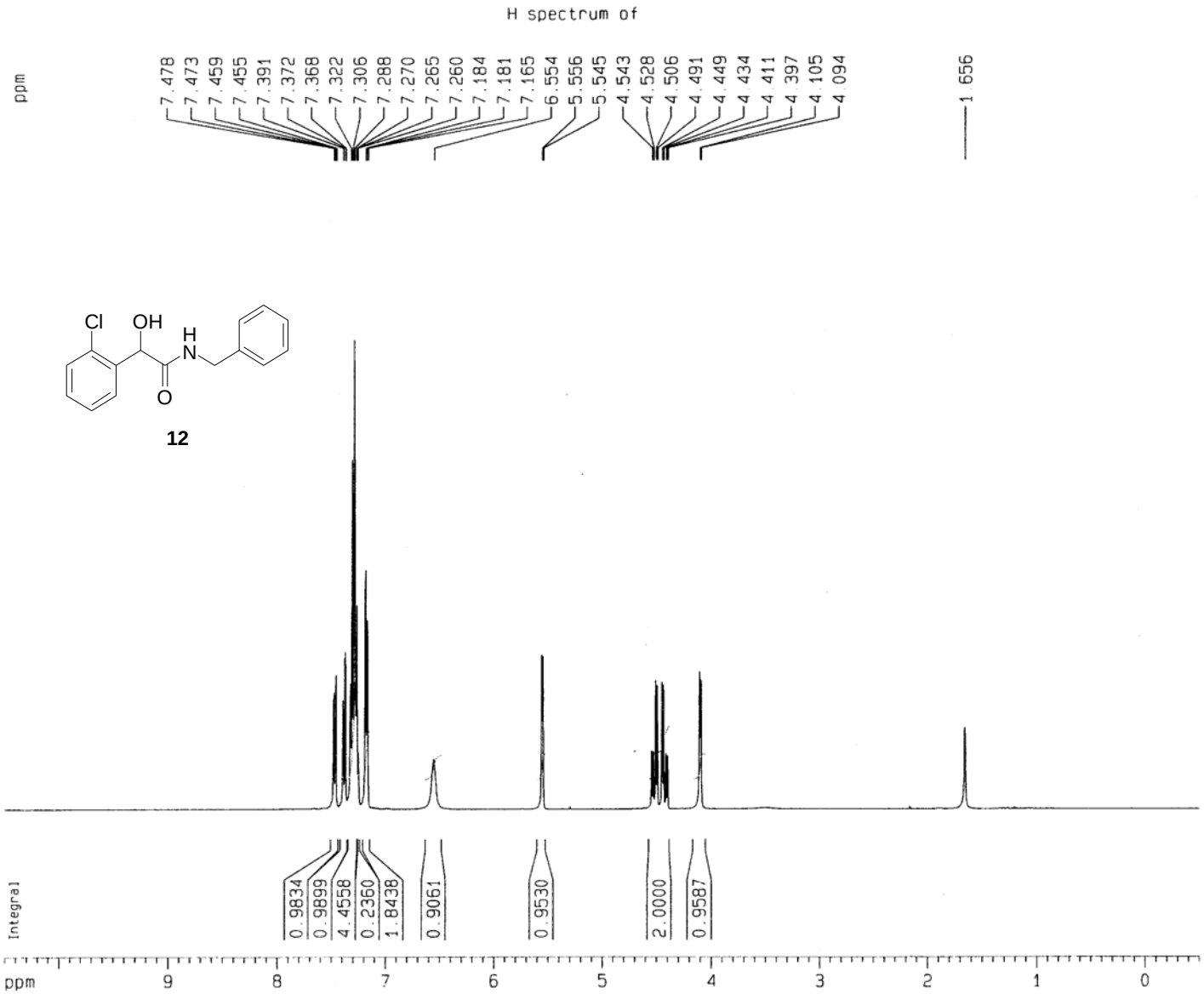



```
Current Data Parameters
NAME      4ClmedelicBnamide
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_            20050225
Time                23.24
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   345
DS                     0
SWH            25125.629 Hz
FIDRES          0.383387 Hz
AQ             1.3042164 sec
RG                  4096
DW                 19.900 usec
DE                  6.50 usec
TE                 300.0 K
D1             1.20000005 sec
d11            0.03000000 sec
d12            0.00002000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                  10.80 usec
PL1                  7.00 dB
SFO1          100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               90.00 usec
PL2                  3.00 dB
PL12                21.83 dB
PL13                24.80 dB
SFO2          400.1319000 MHz

F2 - Processing parameters
SI                  32768
SF            100.6127759 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                  20.00 cm
CY                  10.00 cm
F1P                220.000 ppm
F1               22134.81 Hz
F2P                -10.000 ppm
F2               -1006.13 Hz
PPMCM             11.50000 ppm/cm
HZCM           1157.04686 Hz/cm
```



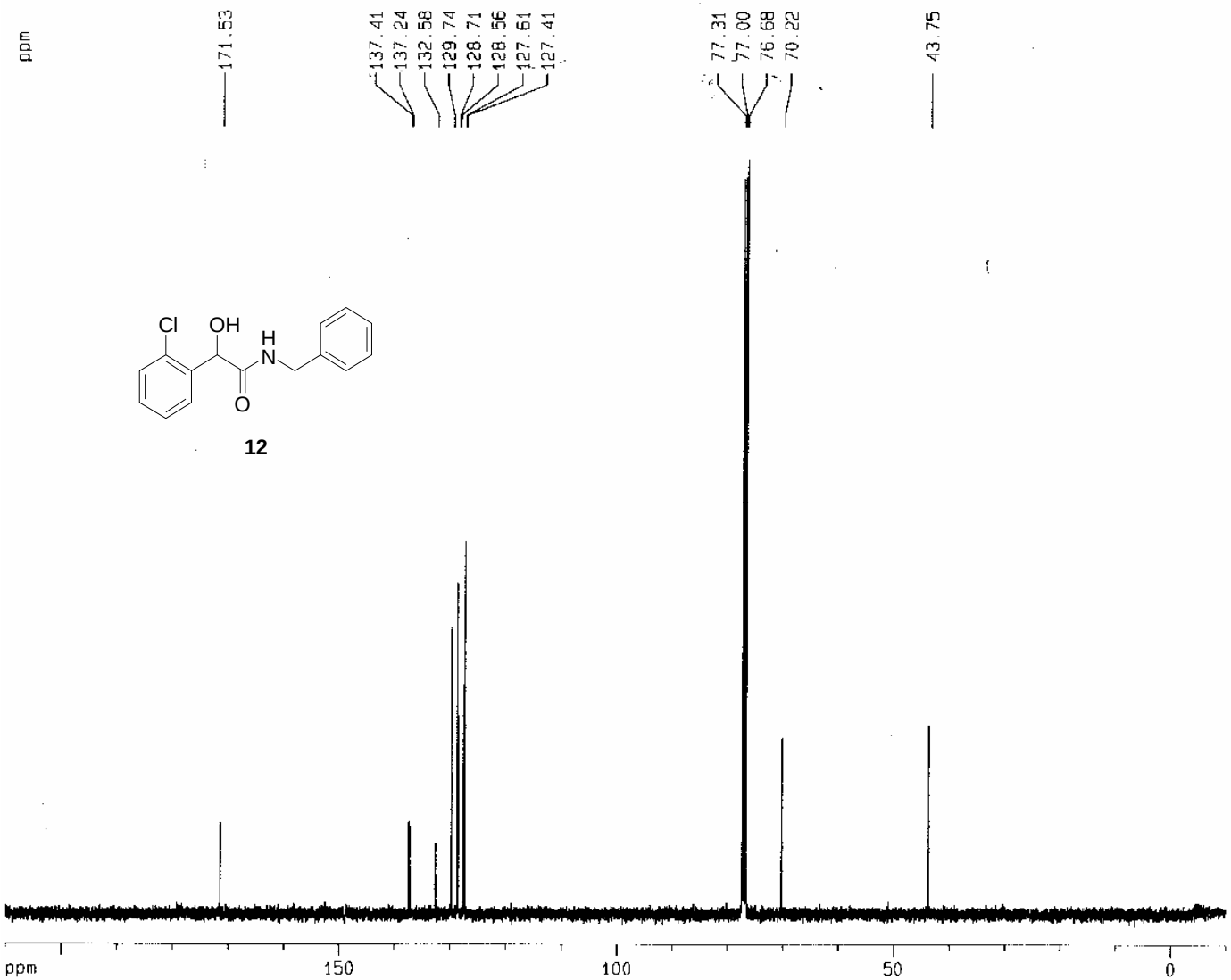

```
Current Data Parameters
NAME      2-Me-Medaliamide
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_            20050213
Time               23.40
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ             1.3664756 sec
RG                  90.5
DW                83.400 usec
DE                 6.50 usec
TE                300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.10 usec
PL1                3.00 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300088 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 10.50 cm
F1P               10.500 ppm
F1               4201.37 Hz
F2P               -0.500 ppm
F2              -200.06 Hz
PPMCM           0.55000 ppm/cm
HZCM          220.07150 Hz/cm
```


C13 spectrumnuntoeqz : spectrum of
ppm
172.63
137.69
137.44
136.77
130.92
128.57
128.45
127.53
127.50
127.44
126.16
127.50
127.44
126.16
77.32
77.00
76.68
71.92
43.22
19.20
OH
H
N
O
11
ppm
200
150
100
50
0

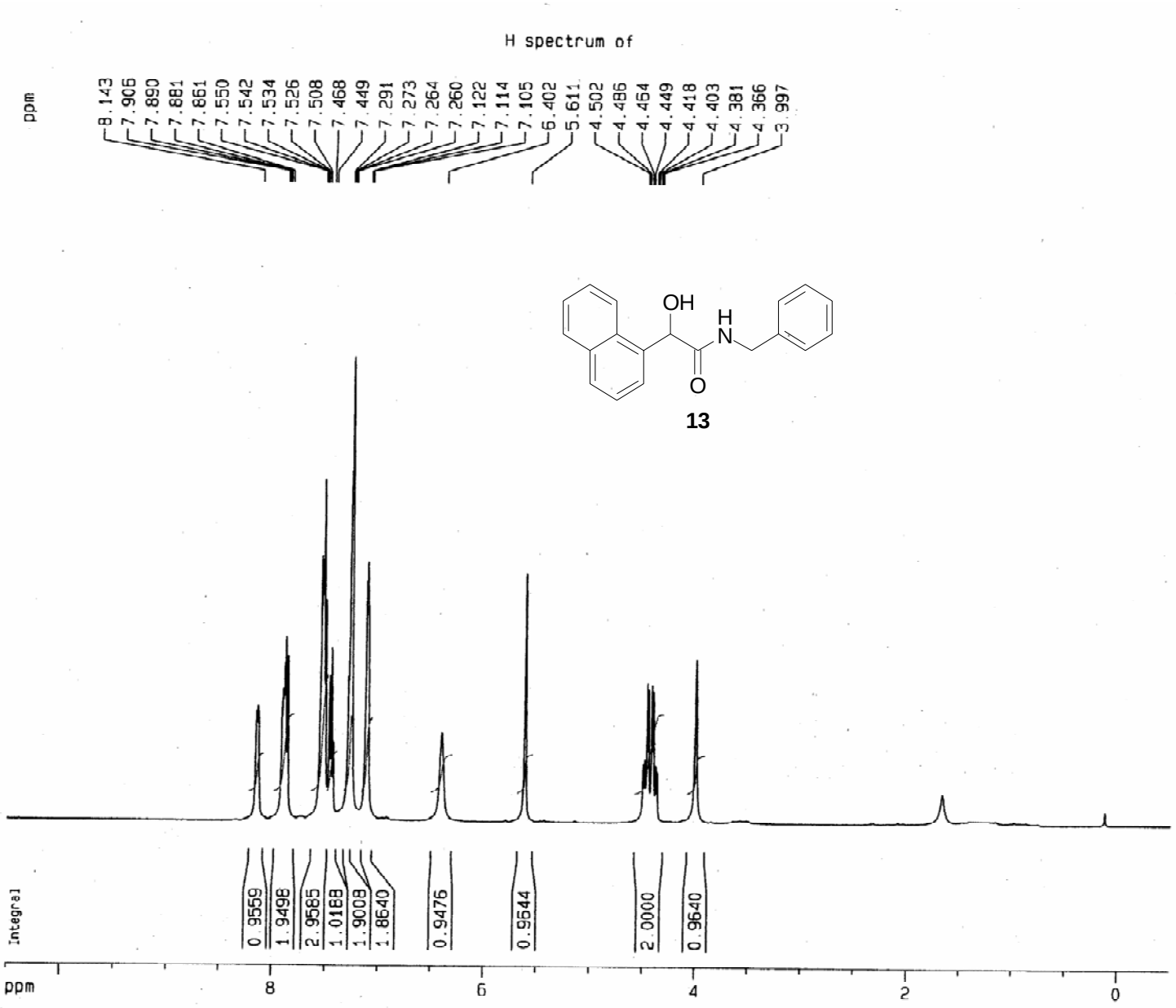



```
Current Data Parameters
NAME      050520.2-Cl-amide
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_            20050520
Time               15.07
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ             1.3664756 sec
RG                 161.3
DW                83.400 usec
DE                 6.50 usec
TE                300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.10 usec
PL1                3.00 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300099 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                  8.00 cm
F1P               10.500 ppm
F1               4201.37 Hz
F2P               -0.500 ppm
F2               -200.07 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07152 Hz/cm
```

C13 spectrum of

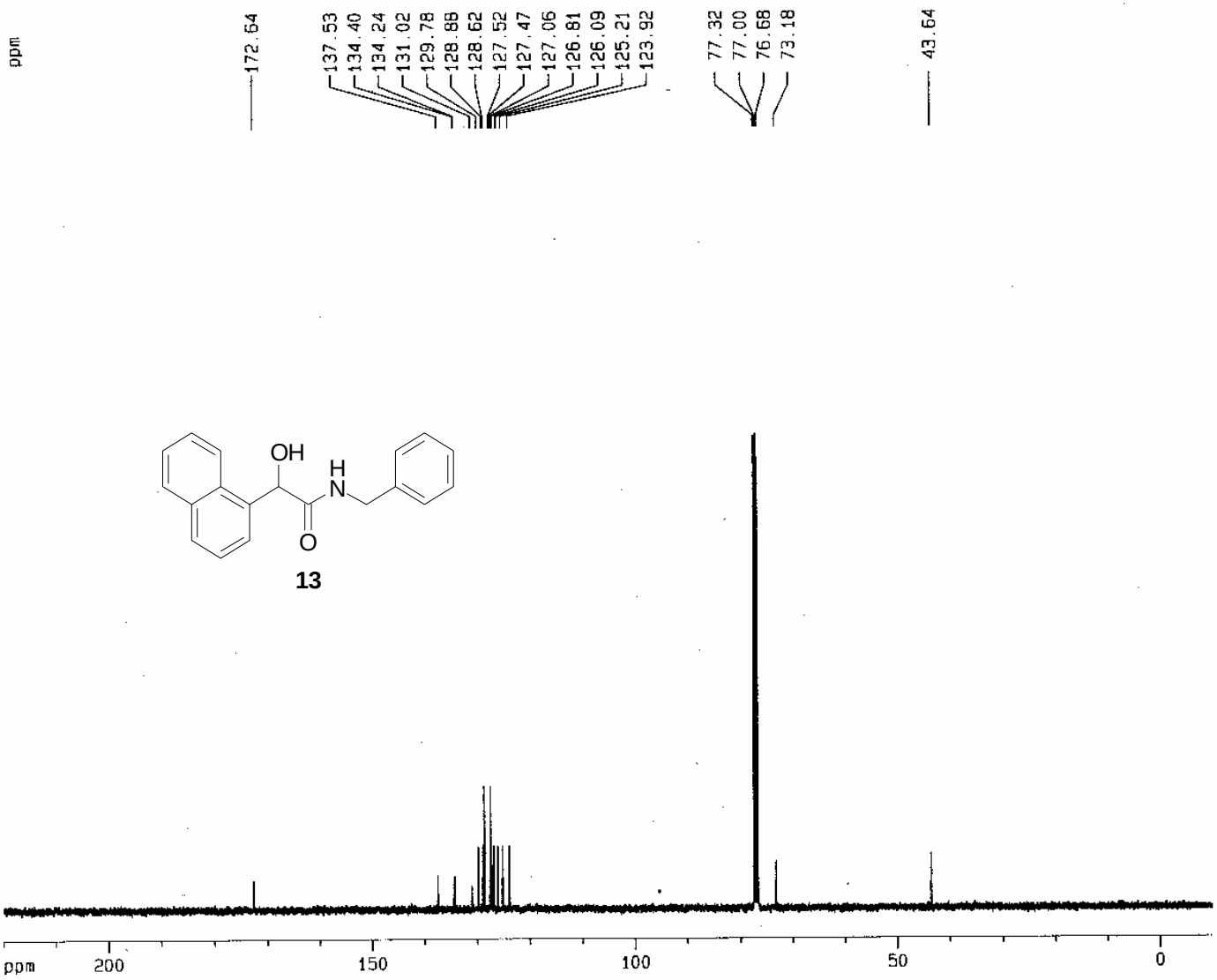



```
Current Data Parameters
NAME      0504122chloroamide
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_            20050412
Time               18.03
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  220
DS                    0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ            1.3042164 sec
RG                 4096
DW               19.900 usec
DE                6.50 usec
TE               300.0 K
D1            1.20000005 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.80 usec
PL1                 7.00 dB
SFO1         100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 3.00 dB
PL12               21.83 dB
PL13               24.80 dB
SFO2         400.1319000 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127744 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 12.50 cm
F1P               210.000 ppm
F1              21128.68 Hz
F2P               -10.000 ppm
F2              -1006.13 Hz
PPMCM            11.00000 ppm/cm
HZCM          1106.74048 Hz/cm
```

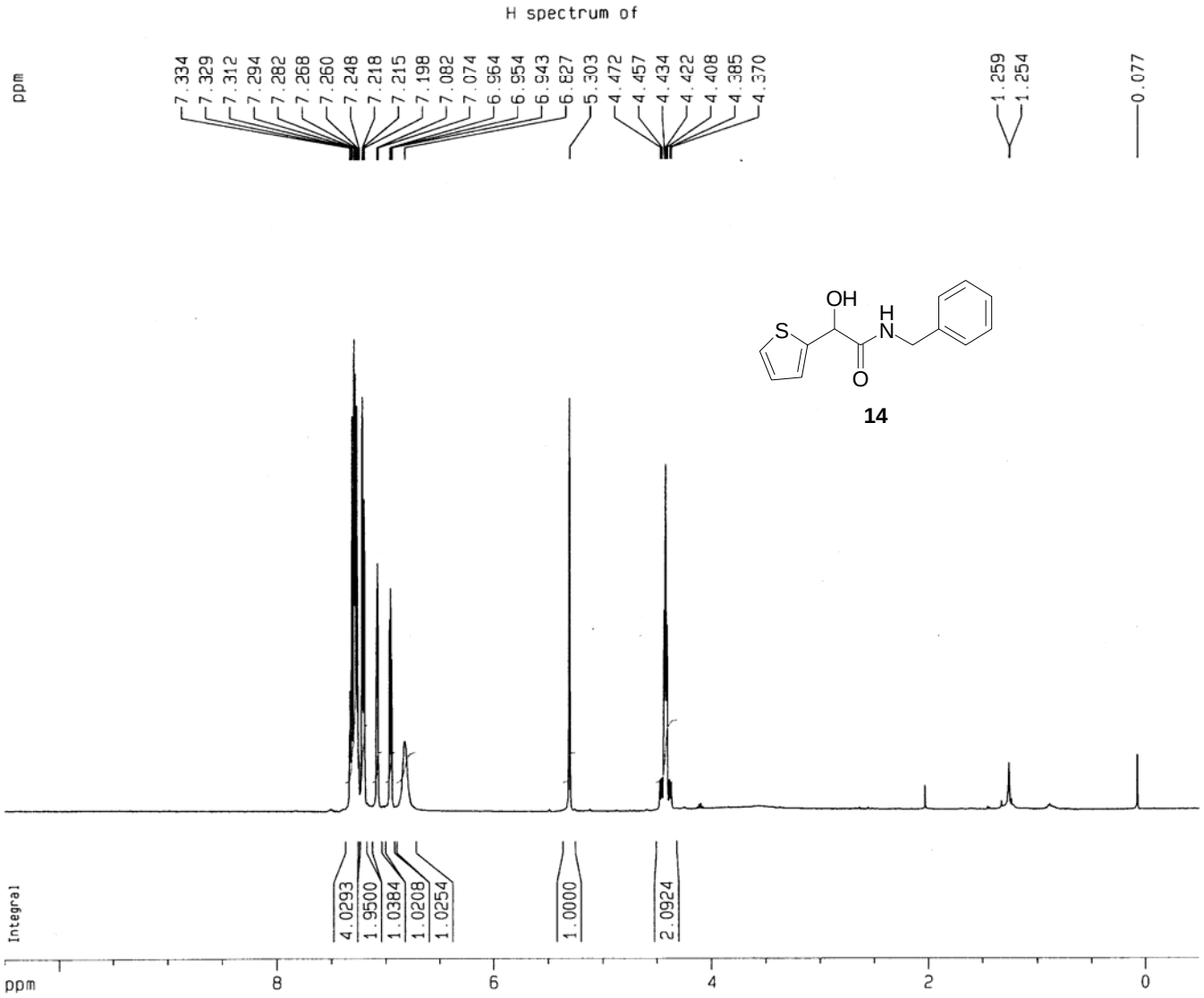



```
Current Data Parameters
NAME      050413.1naphamide
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_            20050414
Time                17.47
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ             1.3664756 sec
RG                 143.7
DW                83.400 usec
DE                  6.50 usec
TE                 300.0 K
D1             1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.10 usec
PL1                3.00 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1299967 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                  8.00 cm
F1P               10.500 ppm
F1               4201.37 Hz
F2P               -0.500 ppm
F2               -200.06 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07150 Hz/cm
```

C13 spectrum of

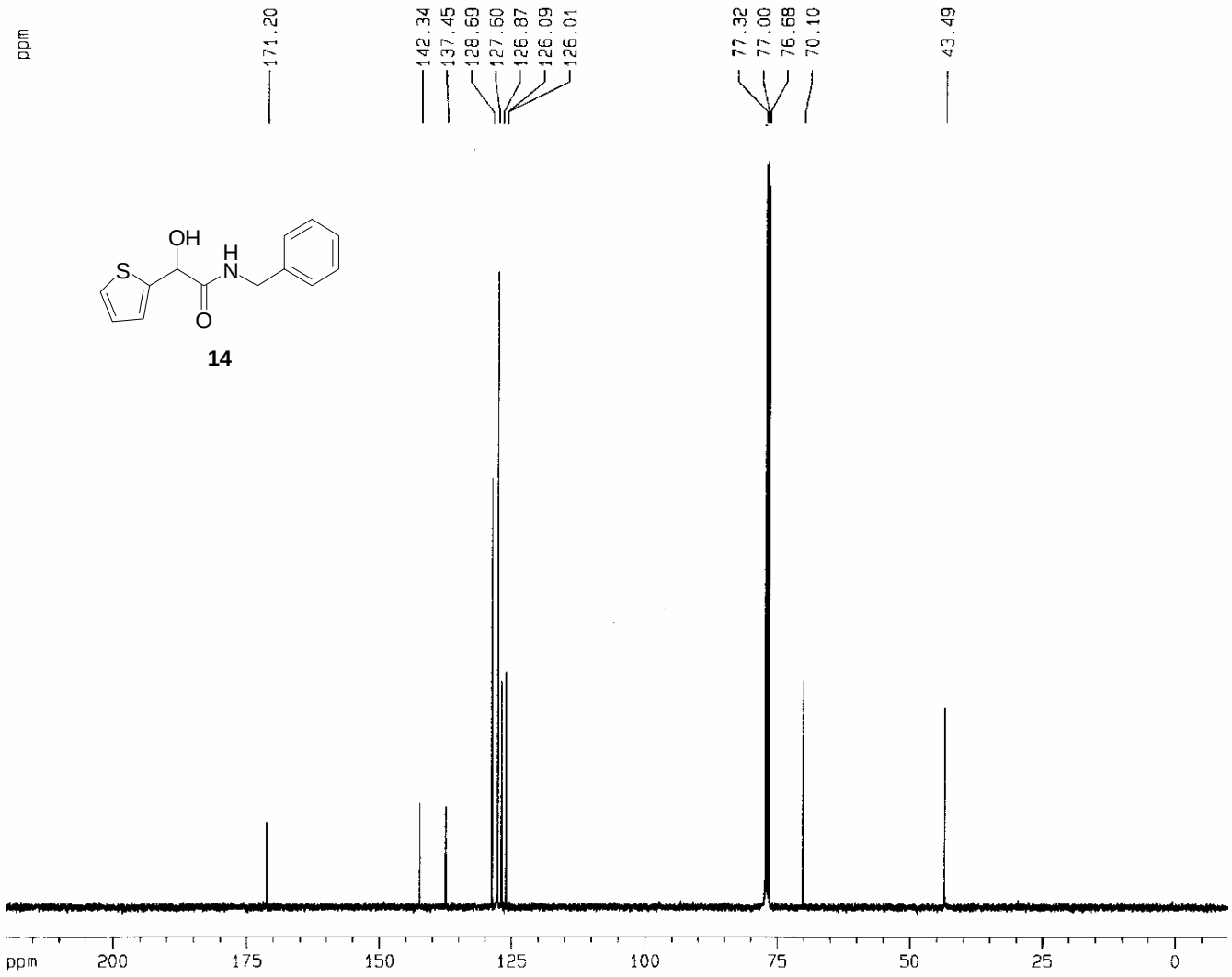



```
Current Data Parameters
NAME      050415.1-naph-amide
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20050415
Time                  19.46
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      234
DS                        0
SWH              25125.629 Hz
FIDRES            0.383387 Hz
AQ               1.3042164 sec
RG                     4096
DW                   19.900 usec
DE                    6.50 usec
TE                   300.0 K
D1               1.20000005 sec
d11              0.03000000 sec
d12              0.00002000 sec

======== CHANNEL f1 ========
NUC1                    13C
P1                    10.80 usec
PL1                    7.00 dB
SFO1            100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                 90.00 usec
PL2                    3.00 dB
PL12                  21.83 dB
PL13                  24.80 dB
SFO2            400.1319000 MHz

F2 - Processing parameters
SI                     32768
SF              100.6127729 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40

1D NMR plot parameters
CX                     20.00 cm
CY                      8.00 cm
F1P                   220.000 ppm
F1                  22134.81 Hz
F2P                  -10.000 ppm
F2                  -1006.13 Hz
PPMCM                11.50000 ppm/cm
HZCM              1157.04688 Hz/cm
```

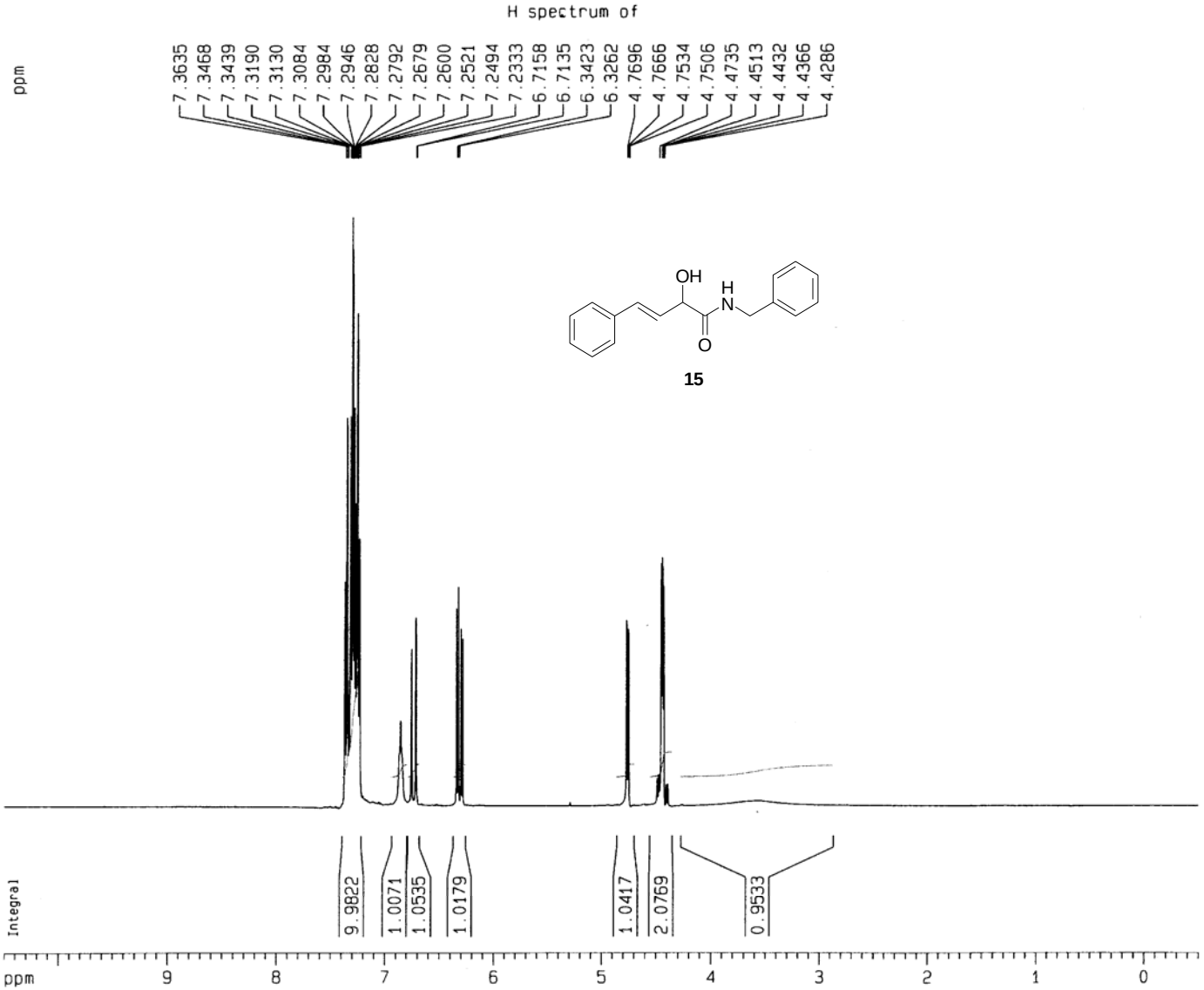



```
Current Data Parameters
NAME          BnNthiophen
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20050213
Time                14.34
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  16384
SOLVENT             CDCl3
NS                      4
DS                      0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ             1.3664756 sec
RG                  143.7
DW                 83.400 usec
DE                   6.50 usec
TE                  300.0 K
D1             1.50000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.10 usec
PL1                  3.00 dB
SFO1          400.1326008 MHz

F2 - Processing parameters
SI                  16384
SF            400.1300088 MHz
WDW                    EM
SSB                     0
LB                   0.10 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
CY                   8.00 cm
F1P                 10.500 ppm
F1                4201.37 Hz
F2P                 -0.500 ppm
F2                -200.06 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07150 Hz/cm
```

C13 spectrum of

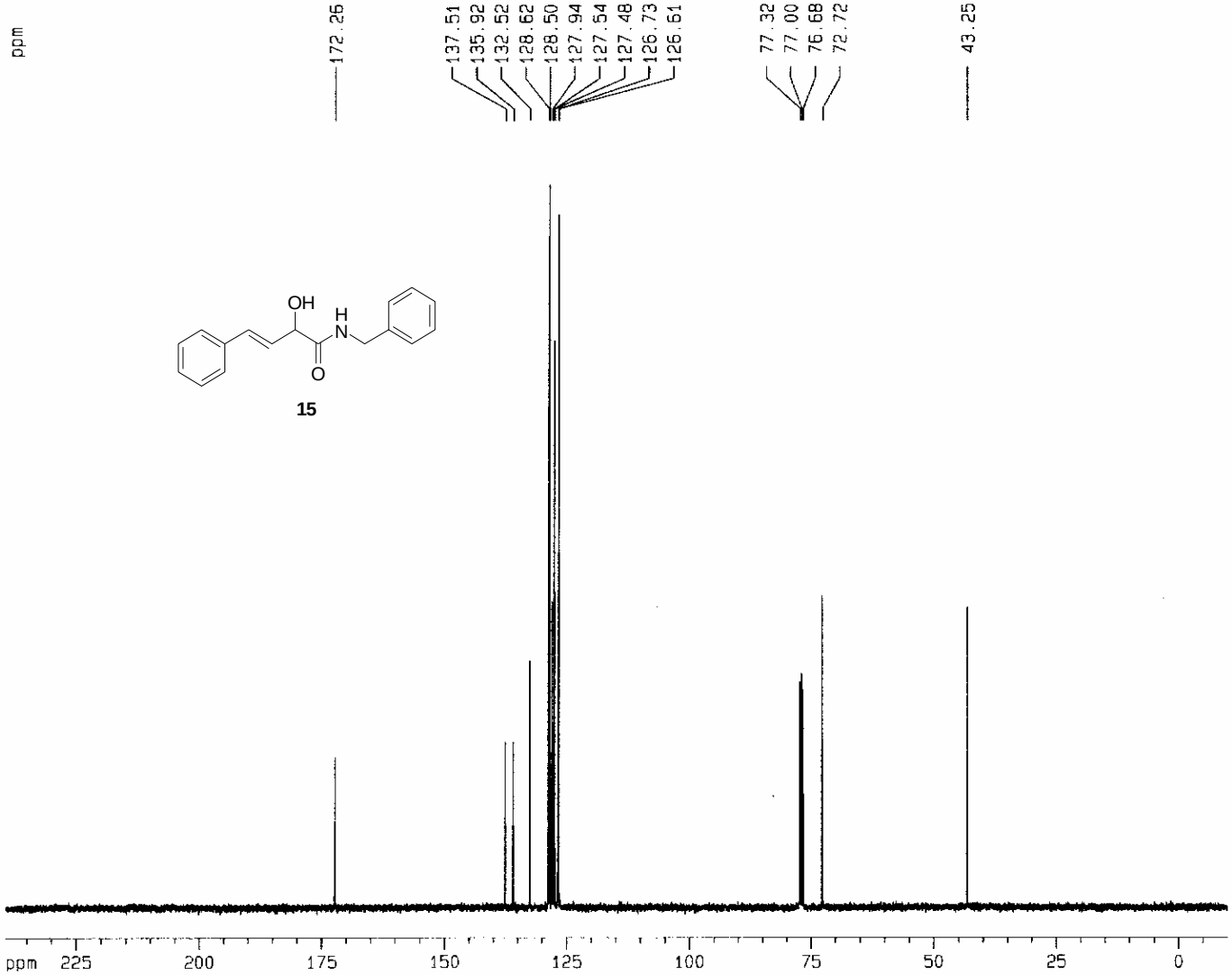



```
Current Data Parameters
NAME          BnNthiophen
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20050213
Time               14.42
INSTRUM            spect
PROBHD   5 mm 680 BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  941
DS                    0
SWH            25125.629 Hz
FIDRES          0.383387 Hz
AQ             1.3042164 sec
RG                 4096
DW                19.900 usec
DE                 6.50 usec
TE                300.0 K
D1            1.20000005 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.80 usec
PL1                7.00 dB
SFO1         100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.80 dB
SFO2         400.1319000 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127752 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 12.50 cm
F1P             220.000 ppm
F1              22134.81 Hz
F2P              -10.000 ppm
F2              -1006.13 Hz
PPMCM            11.50000 ppm/cm
HZCM          1157.04688 Hz/cm
```



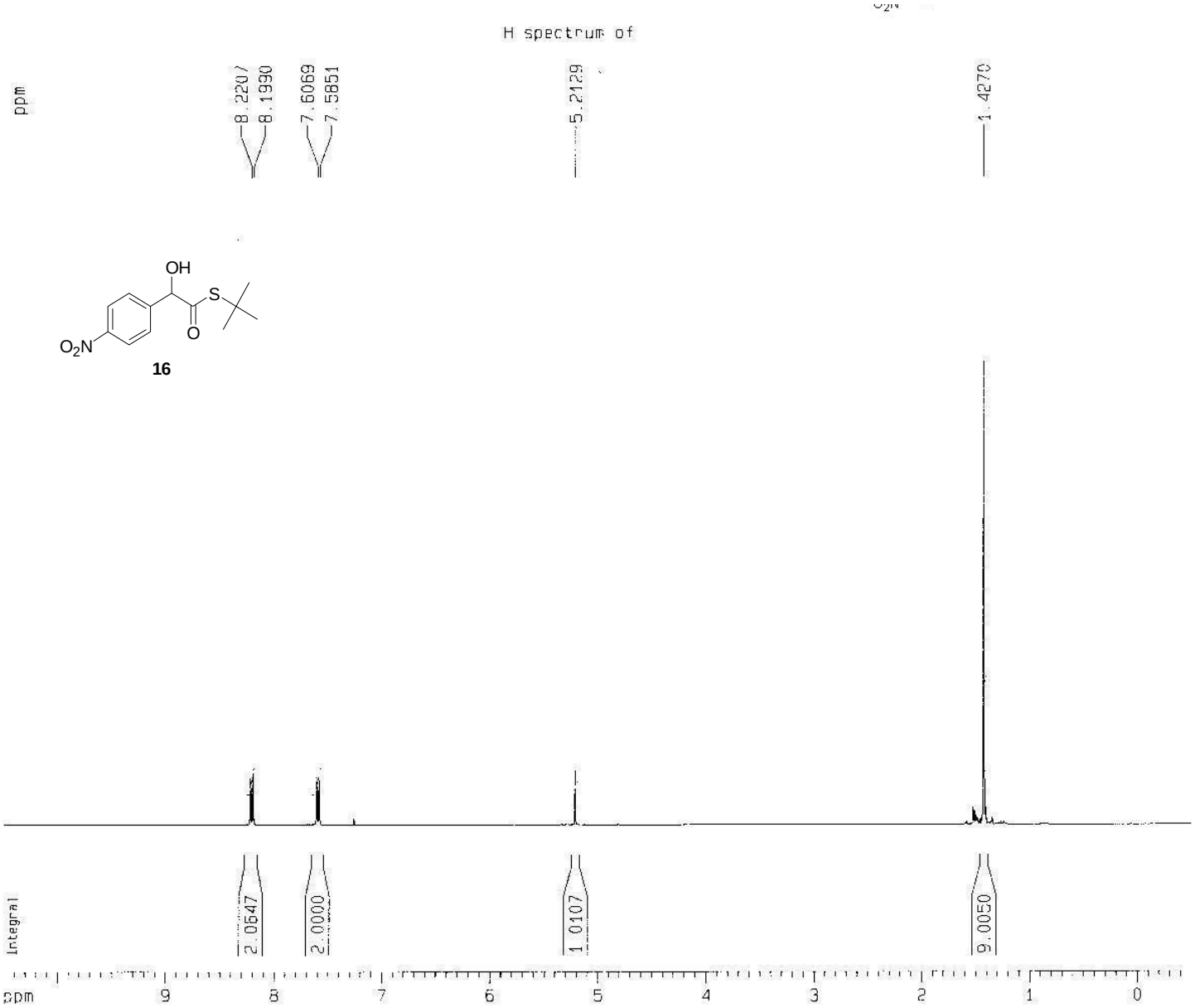

```
Current Data Parameters
NAME      cinamylmedelate
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20050404
Time               12.06
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ            1.3664756 sec
RG                   128
DW                83.400 usec
DE                  6.50 usec
TE                 300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.10 usec
PL1                 3.00 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300091 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 10.00 cm
F1P               10.500 ppm
F1               4201.37 Hz
F2P               -0.500 ppm
F2               -200.07 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07152 Hz/cm
```

C13 spectrum of

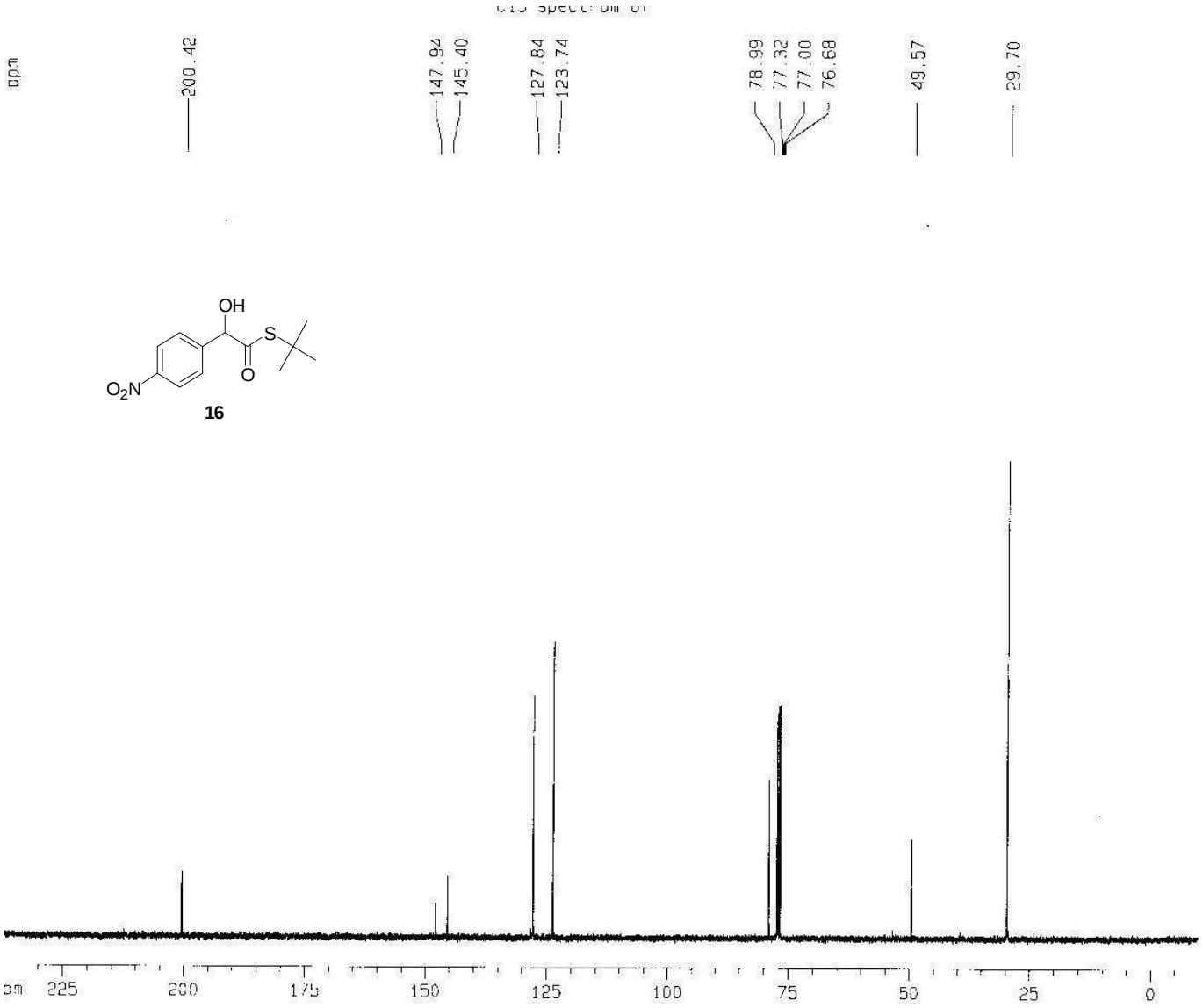



```
Current Data Parameters
NAME      cinamylmedelate
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_           20050404
Time               11.45
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  181
DS                    0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ            1.3042164 sec
RG                 4096
DW               19.900 usec
DE                6.50 usec
TE               300.0 K
D1           1.20000005 sec
d11          0.03000000 sec
d12          0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.80 usec
PL1                7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2            90.00 usec
PL2               3.00 dB
PL12             21.83 dB
PL13             24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                32768
SF          100.6127836 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                12.00 cm
F1P              240.000 ppm
F1             24147.07 Hz
F2P              -10.000 ppm
F2             -1006.13 Hz
PPMCM           12.50000 ppm/cm
HZCM          1257.65979 Hz/cm
```

16

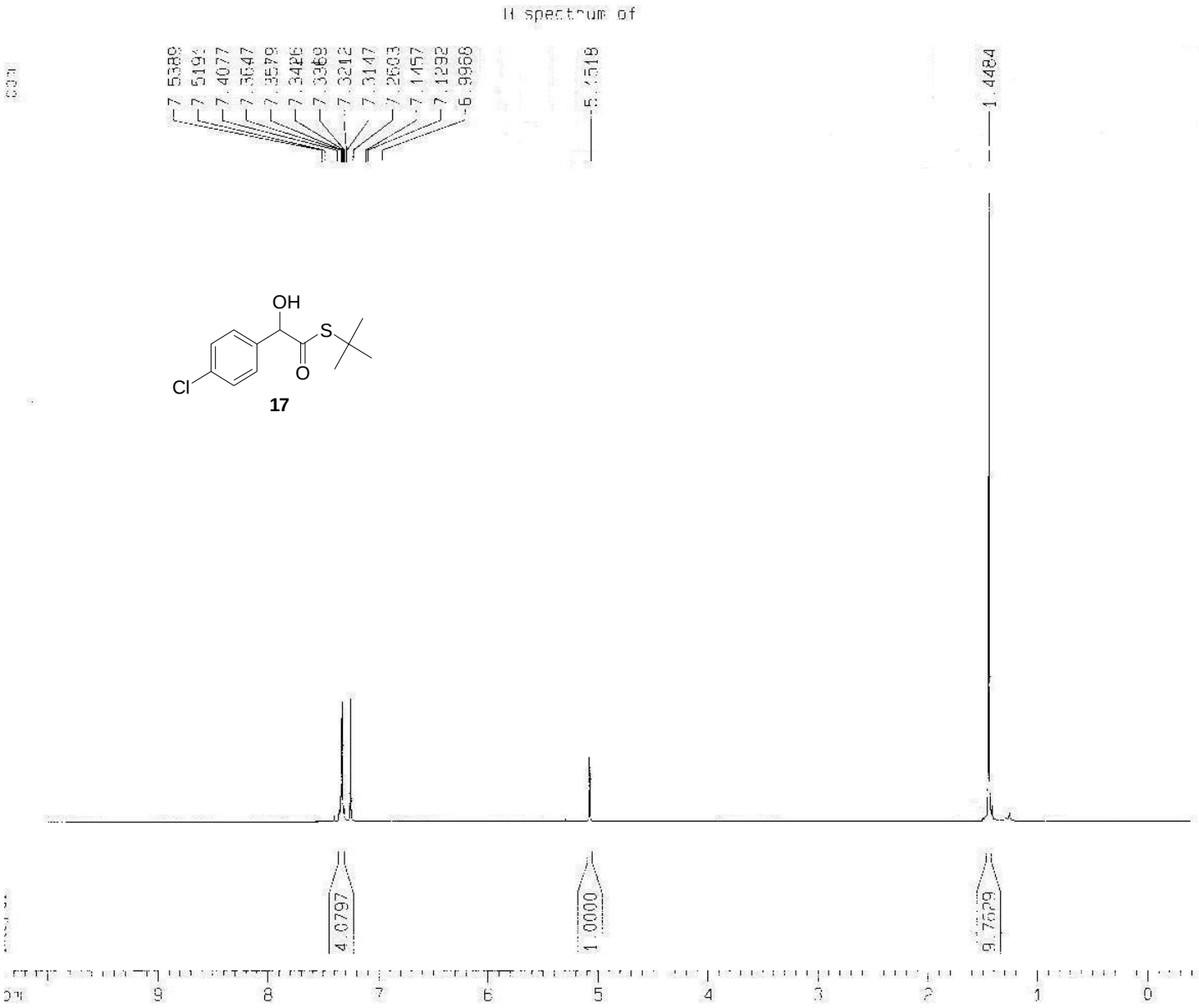



```
NAME        sam-HT-4nitro
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20060309
Time                12.05
INSTRUM             spect
PROBHD   5 mm SBO BB-1H
PULPROG             zg30
TD                  16384
SOLVENT             CDCl3
NS                      1
DS                      0
SWH              5995.204 Hz
FIDRES           0.365918 Hz
AQ               1.3664756 sec
RG                   71.8
DW                 83.400 usec
DE                   6.50 usec
TE                  300.0 K
D1             1.50000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.10 usec
PL1                  3.00 dB
SFO1          400.1326008 MHz

F2 - Processing parameters
SI                  16384
SF            400.1300095 MHz
WDW                    EM
SSB                     0
LB                   0.10 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
CY                   8.00 cm
F1P                 10.500 ppm
F1                4201.37 Hz
F2P                 -0.500 ppm
F2                -200.07 Hz
PPMCM             0.55000 ppm/cm
HZCM            220.07152 Hz/cm
```

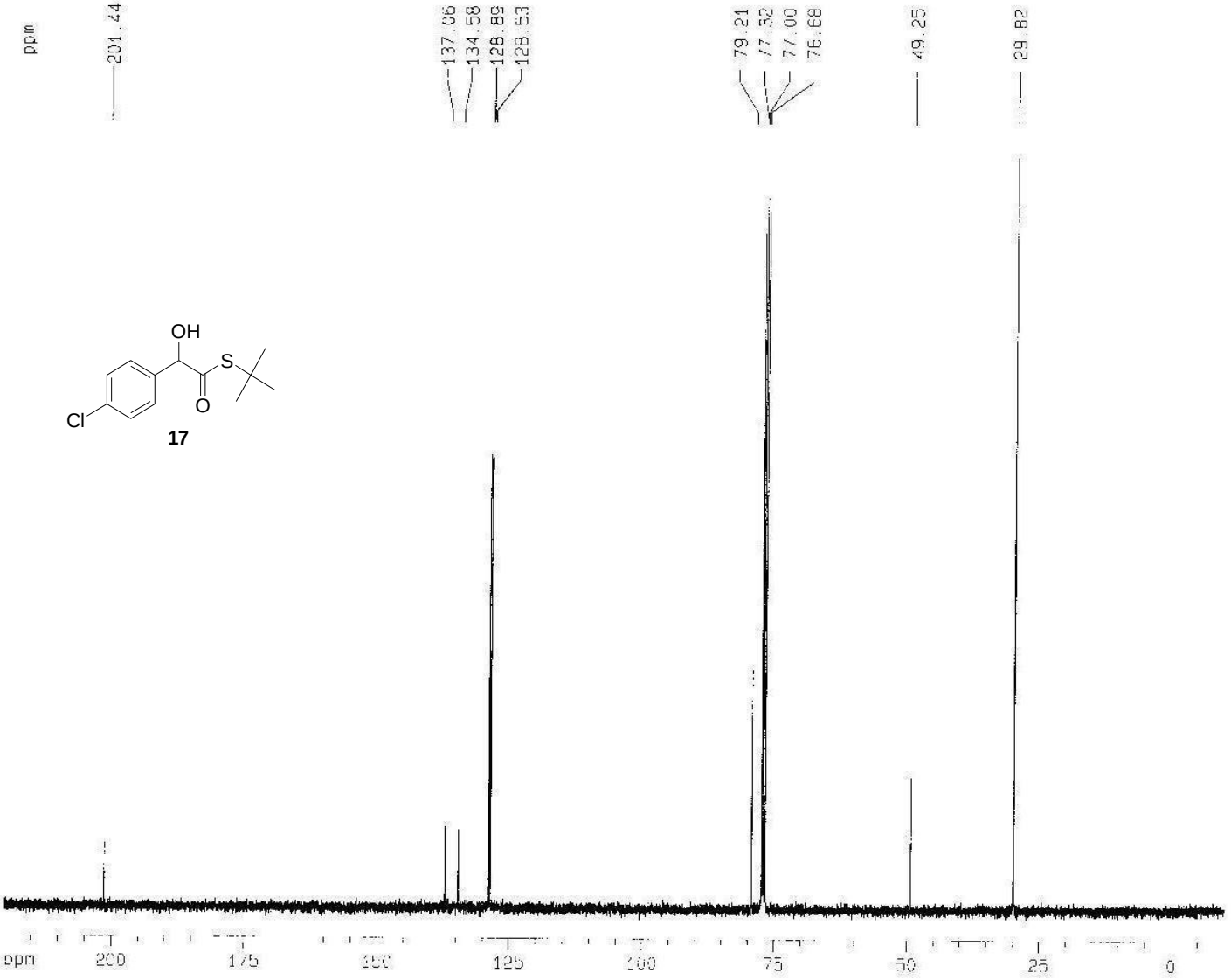


16

```
Current Data Parameters
NAME        sam-HT-4nitro
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20050309
Time               12.09
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   88
DS                    0
SWH            25125.629 Hz
FIDRES          0.383387 Hz
AQ             1.3042164 sec
RG                 8192
DW                19.900 usec
DE                 6.50 usec
TE                300.0 K
D1             1.20000005 sec
d11            0.03000000 sec
d12            0.00002000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.80 usec
PL1                 7.00 dB
SFO1         100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 3.00 dB
PL12               21.83 dB
PL13               24.60 dB
SFO2         400.1319000 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127759 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                  8.00 cm
F1P              239.397 ppm
F1             24086.36 Hz
F2P              -10.000 ppm
F2             -1006.13 Hz
PPMCM            12.46983 ppm/cm
HZCM           1254.82427 Hz/cm
```

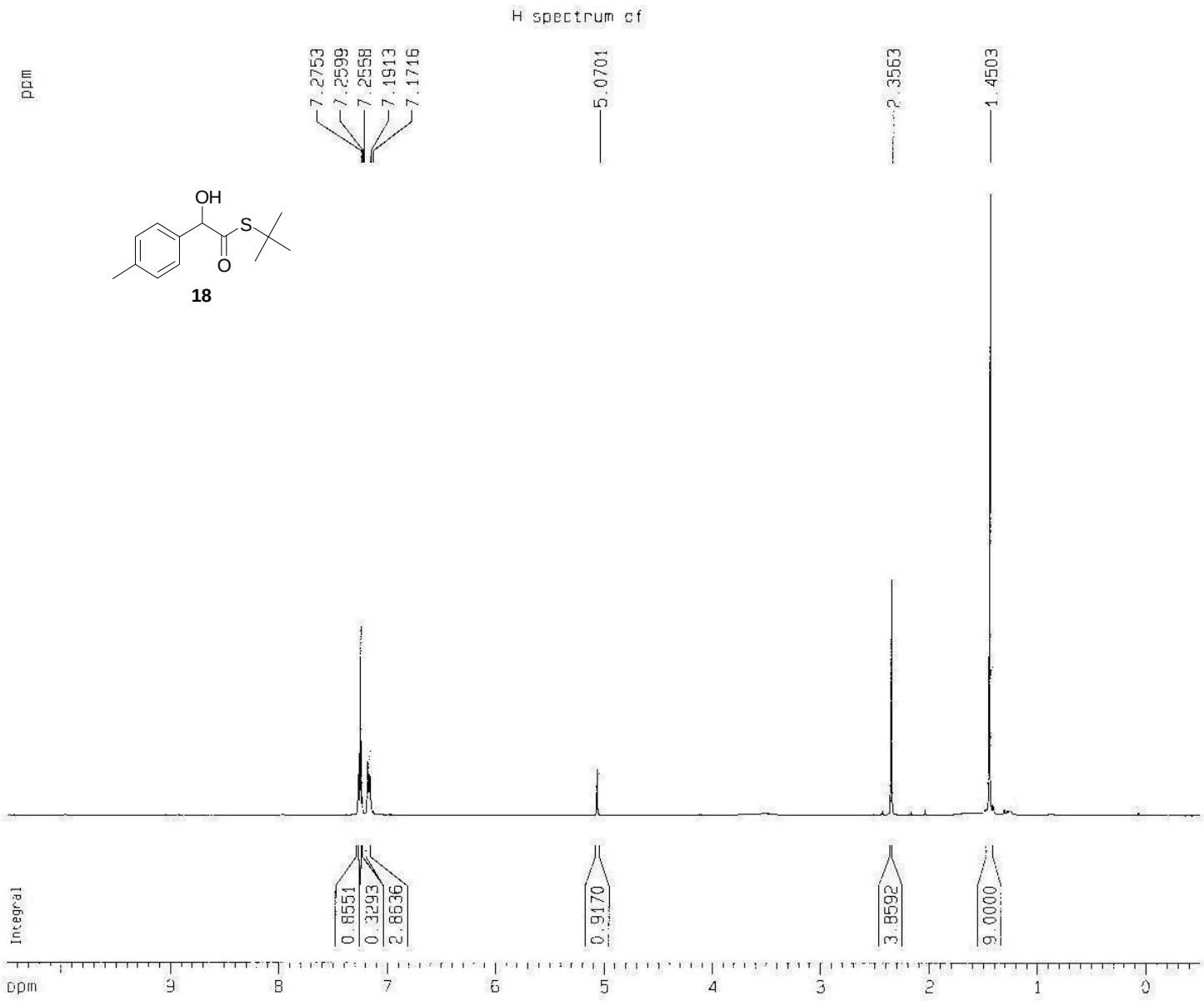



```
NAME                 4-Cl-Cl6
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_             20080218
Time                  11.33
INSTRUM               spect
PROBHD   5 mm BBO BB-H-D
PULPROG                zg30
TD                    16384
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                5995.204 Hz
FIDRES             0.365918 Hz
AQ                 1.3664756 sec
RG                     645.1
DW                    83.400 usec
DE                     6.50 usec
TE                     300.0 K
D1                 1.50000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.10 usec
PL1                     3.00 dB
SFO1             400.1326008 MHz

F2 - Processing parameters
SI                    16384
SF               400.1300095 MHz
WDW                      EM
SSB                       0
LB                     0.10 Hz
GB                        0
PC                     1.00

1D NMR plot parameters
CX                    20.00 cm
CY                    10.50 cm
F1P                 10.500 ppm
F1                  4201.37 Hz
F2P                 -0.500 ppm
F2                  -200.07 Hz
PPMCM               0.55000 ppm/cm
HZCM              220.07152 Hz/cm
```

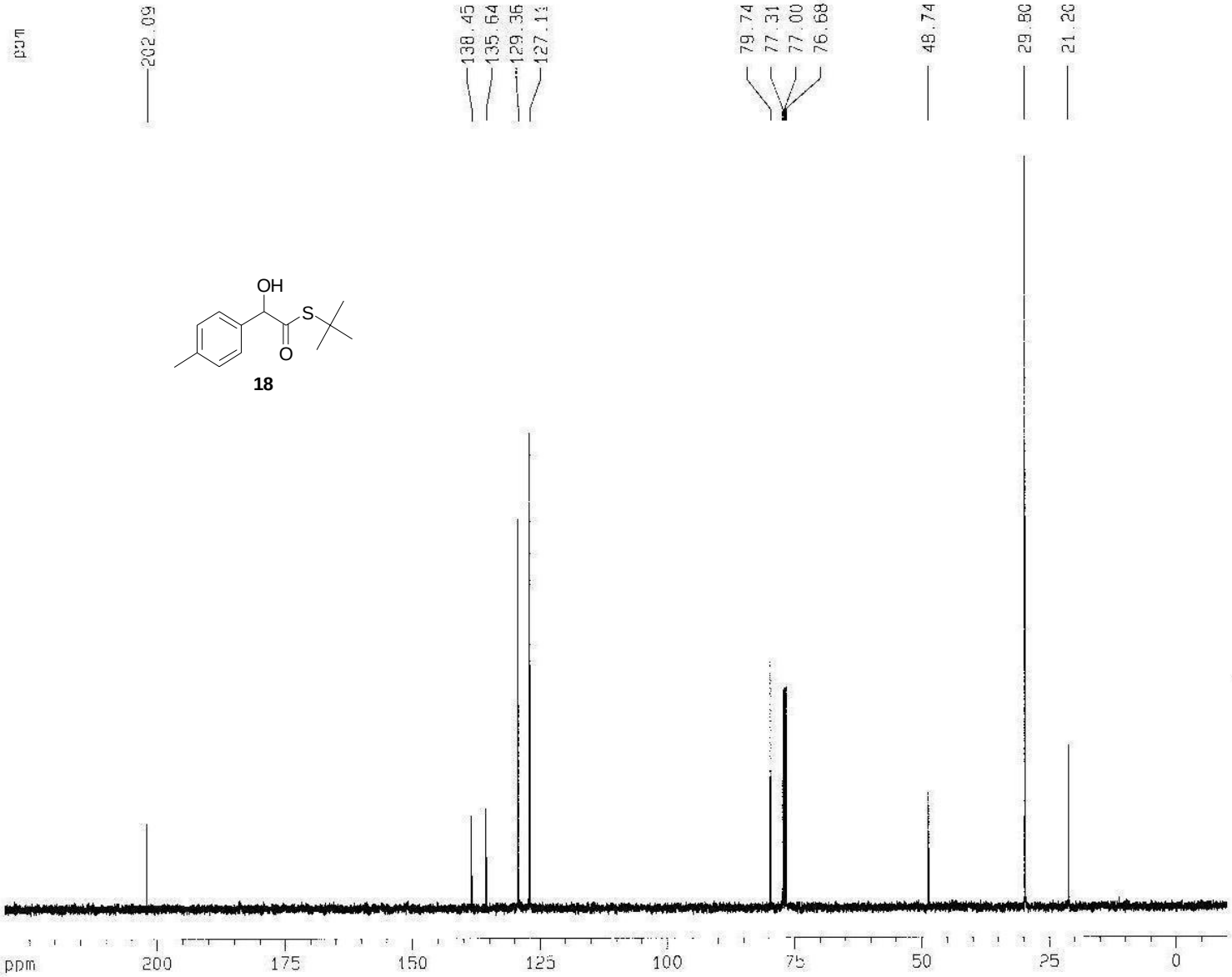



```
Current Data Parameters
NAME      sam-4-Chloro H1
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date            20060412
Time               22.40
INSTRUM            spect
PROBHD   5 mm BBO BB 1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  729
DS                    0
SWH           25125.628 Hz
FIDRES         0.383387 Hz
AQ             1.3042164 sec
RG                 8192
DW               19.900 usec
DE                6.50 usec
TE               300.0 K
D1            1.20000005 sec
D11           0.03000000 sec
D12           0.00002000 sec

====  == CHANNEL f1 ====  ===
NUC1                 13C
P1                10.60 usec
PL1                7.00 dB
SFO1         100.6242995 MHz

====  == CHANNEL f2 ===
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.93 dB
PL13              24.90 dB
SFO2         400.1319000 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127708 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 12.50 cm
F1P             220.000 ppm
F1              22134.81 Hz
F2P              -10.000 ppm
F2              -1006.13 Hz
PPMCM           11.50000 ppm/cm
HZCM          1152.04688 Hz/cm
```

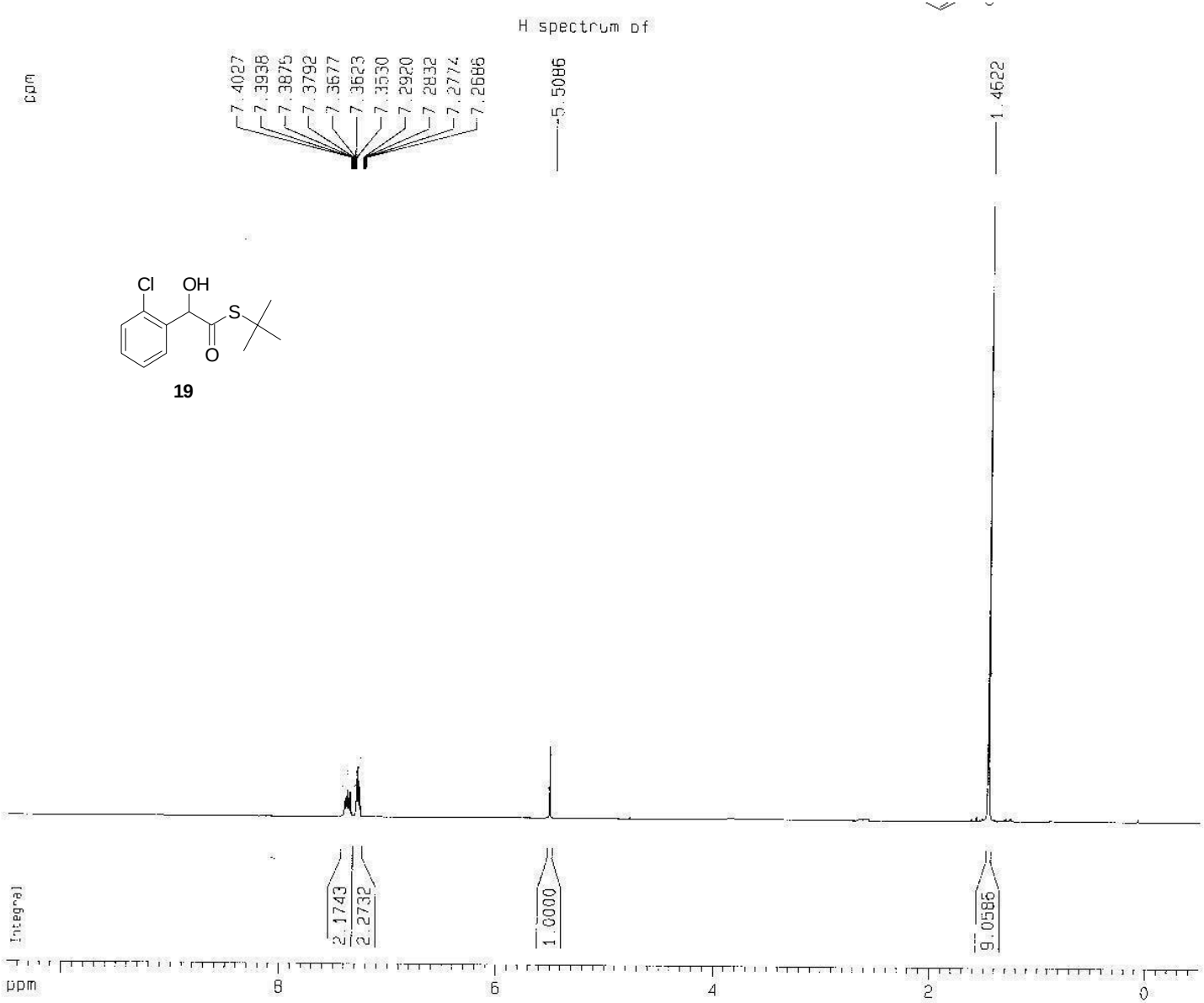
18




```
NAME          sam 4-Me-Hi
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20060311
Time               11.37
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ            1.3664756 sec
RG                 574.7
DW                83.400 usec
DE                  6.50 usec
TE                 300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.10 usec
PL1                 3.00 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300095 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 10.50 cm
F1P               10.500 ppm
F1               4201.37 Hz
F2P               -0.500 ppm
F2               -200.07 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07152 Hz/cm
```

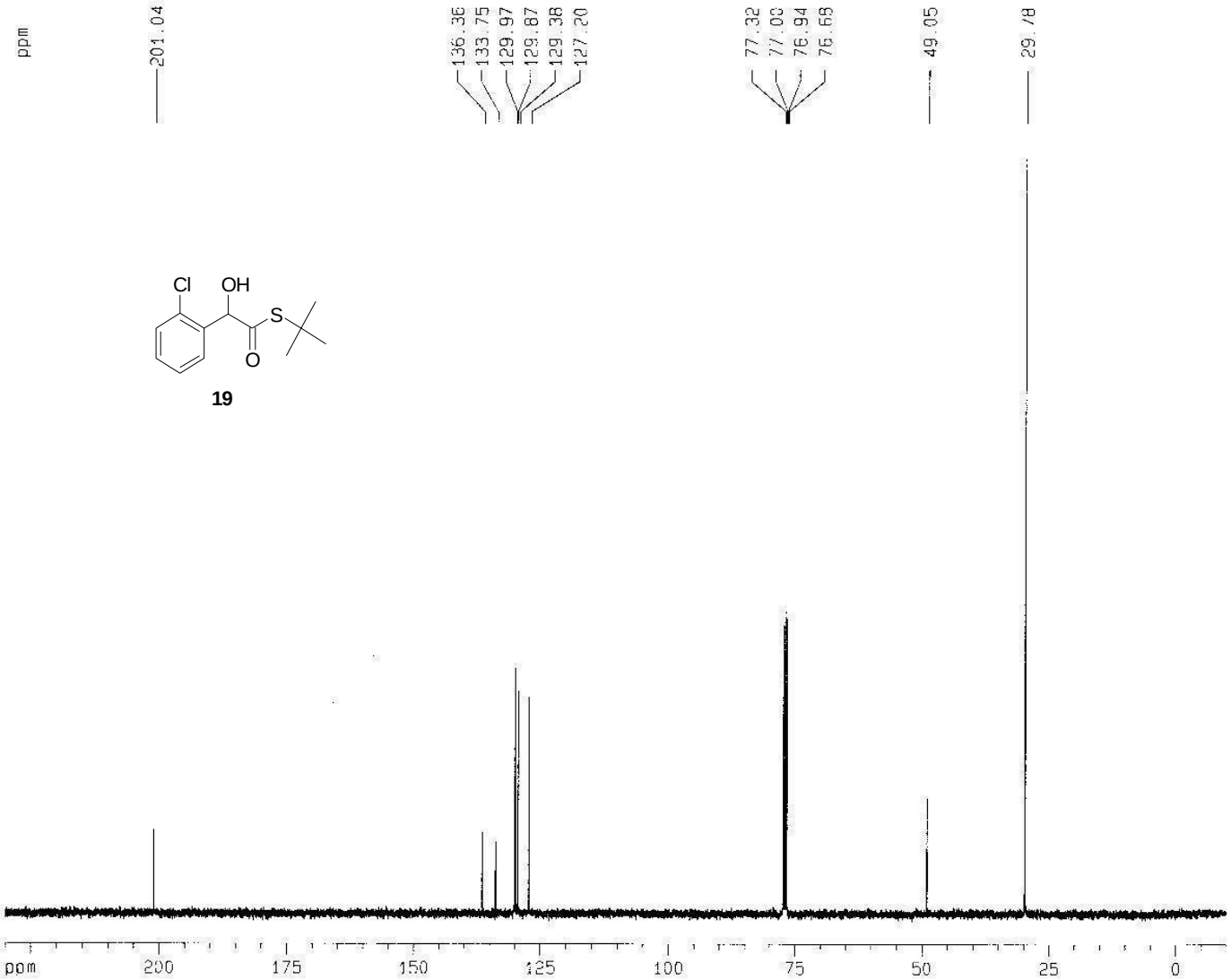



```
Current Data Parameters
NAME          sam-HT-4-Me
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20060311
Time                17.47
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    85
DS                     0
SWH            25125.629 Hz
FIDRES          0.383387 Hz
AQ             1.3042164 sec
RG                 406.4
DW                19.900 usec
DE                 6.50 usec
TE                300.0 K
D1            1.20000005 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.80 usec
PL1                 7.00 dB
SFO1         100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 3.00 dB
PL12               21.83 dB
PL13               24.80 dB
SFO2         400.1319000 MHz

F2 - Processing parameters
SI                 32768
SF            100.6127767 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 12.50 cm
F1P               230.000 ppm
F1              23140.94 Hz
F2P               -10.000 ppm
F2              -1006.13 Hz
PPMCM             12.00000 ppm/cm
HZCM            1207.35327 Hz/cm
```

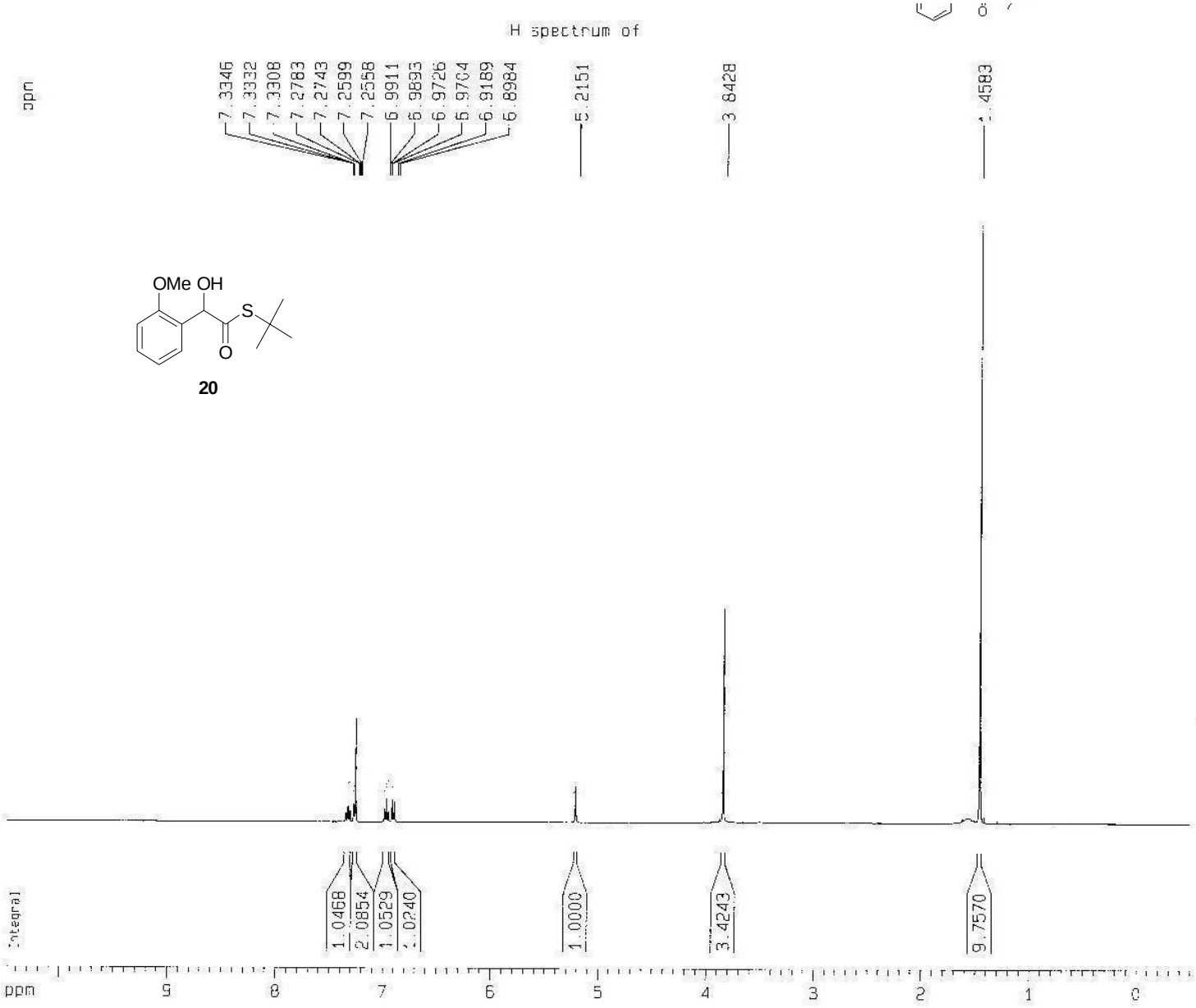



```
NAME          sam-2 Cl-HT
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20060426
Time               18.21
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                    16
DS                     0
SWH            5995.204 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                   114
DW                83.400 usec
DE                 6.50 usec
TE                300.0 K
D1             1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.10 usec
PL1                3.00 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300091 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 10.50 cm
F1P               10.500 ppm
F1               4201.37 Hz
F2P               -0.500 ppm
F2               -200.06 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07150 Hz/cm
```

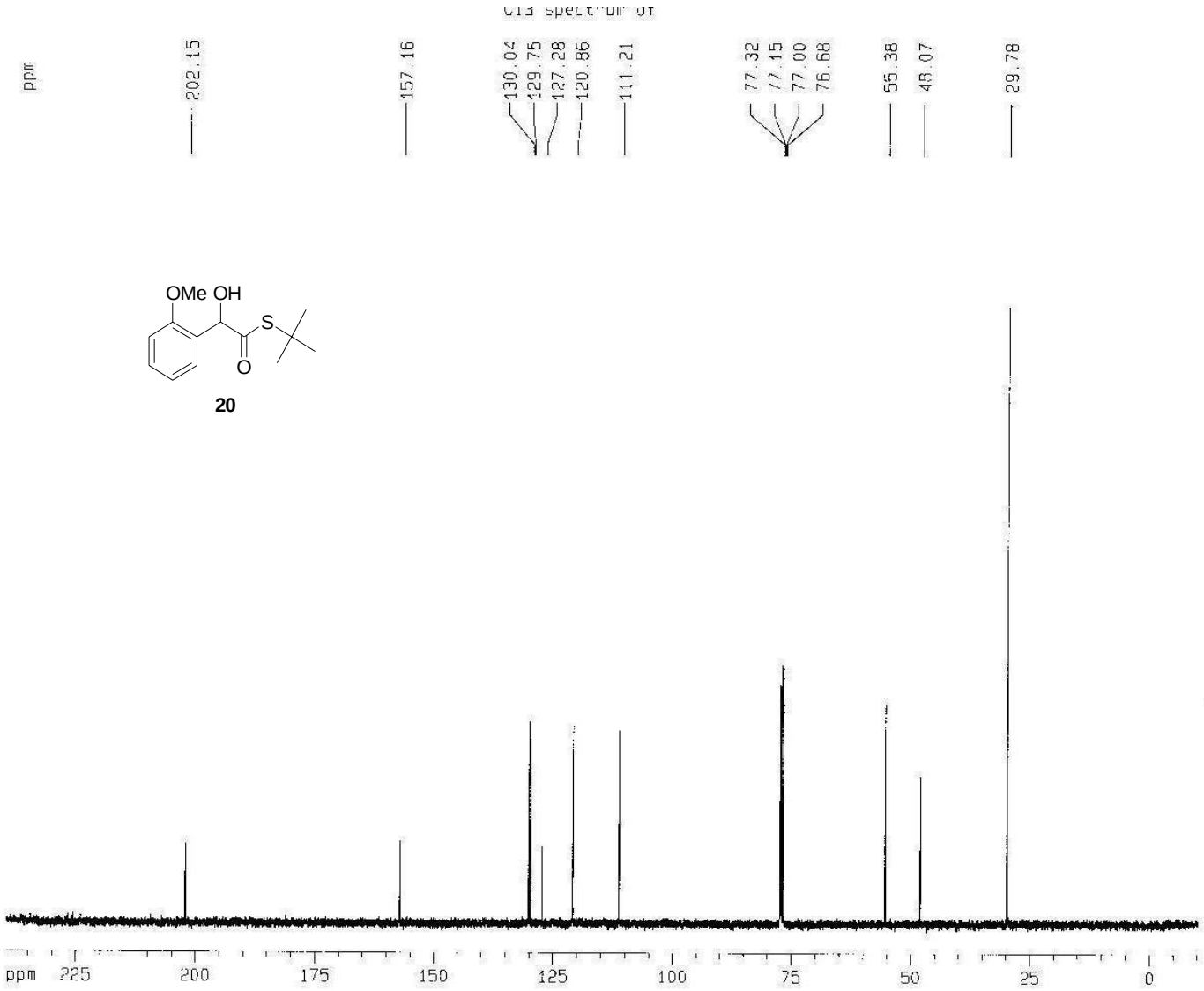
C13 spectrum of



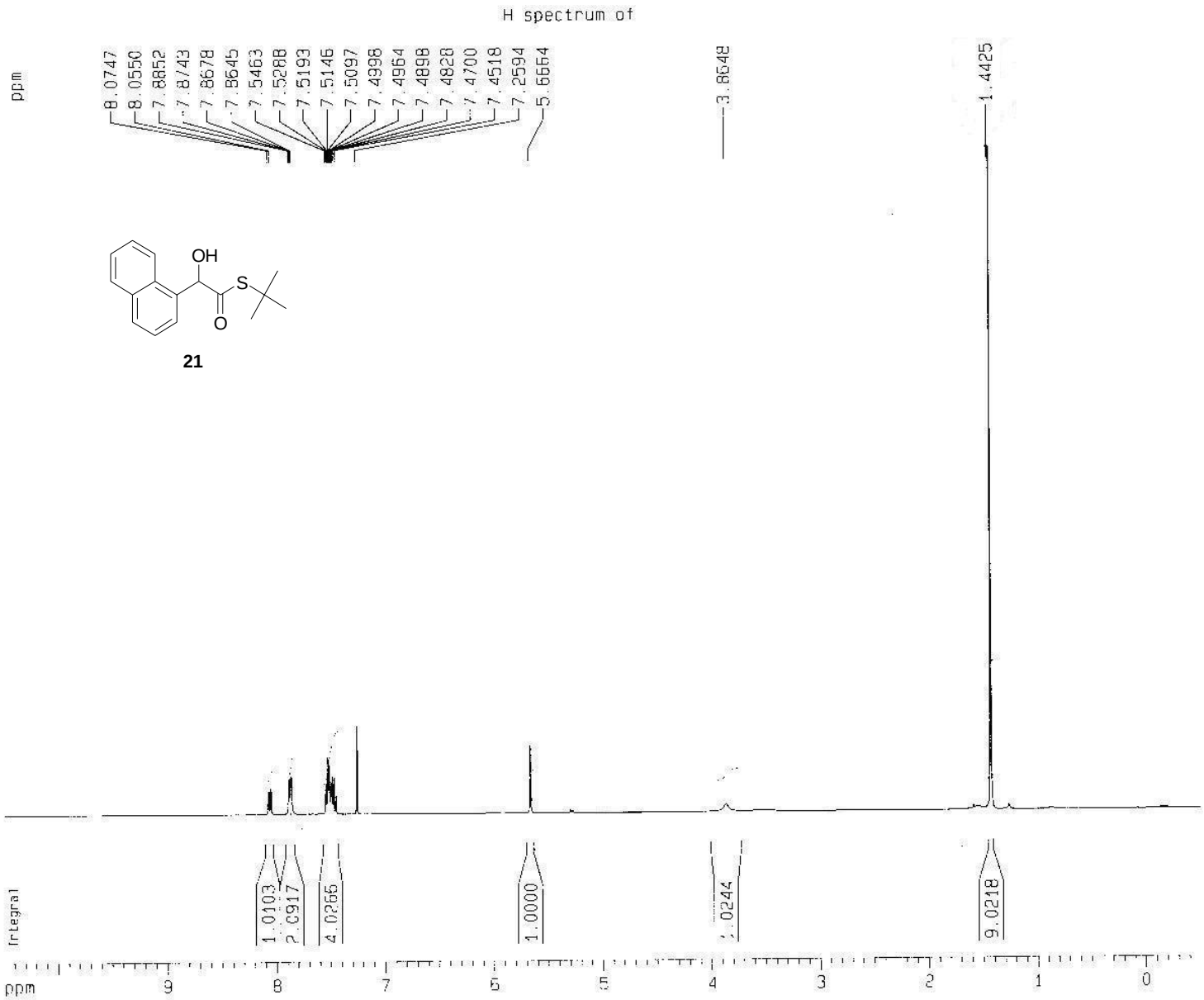

```
Current Data Parameters
NAME          sam-2-C3-HT
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20060426
Time                 19.10
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    122
DS                      0
SWH             25125.629 Hz
FIDRES           0.383397 Hz
AQ              1.3042164 sec
RG                   6192
DW                  19.900 usec
DE                   6.50 usec
TE                  300.0 K
D1              1.20000005 sec
d11             0.03000000 sec
d12             0.00002000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                   10.80 usec
PL1                   7.00 dB
SFO1          100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                   3.00 dB
PL12                 21.83 dB
PL13                 24.80 dB
SFO2          400.1313000 MHz

F2 - Processing parameters
SI                   32768
SF            100.6127752 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40

1D NMR plot parameters
CX                   20.00 cm
CY                   12.50 cm
F1P                 230.000 ppm
F1                 23140.94 Hz
F2P                 -10.000 ppm
F2                 -1006.13 Hz
PPMCM              12.00000 ppm/cm
HZCM             1207.35327 Hz/cm
```



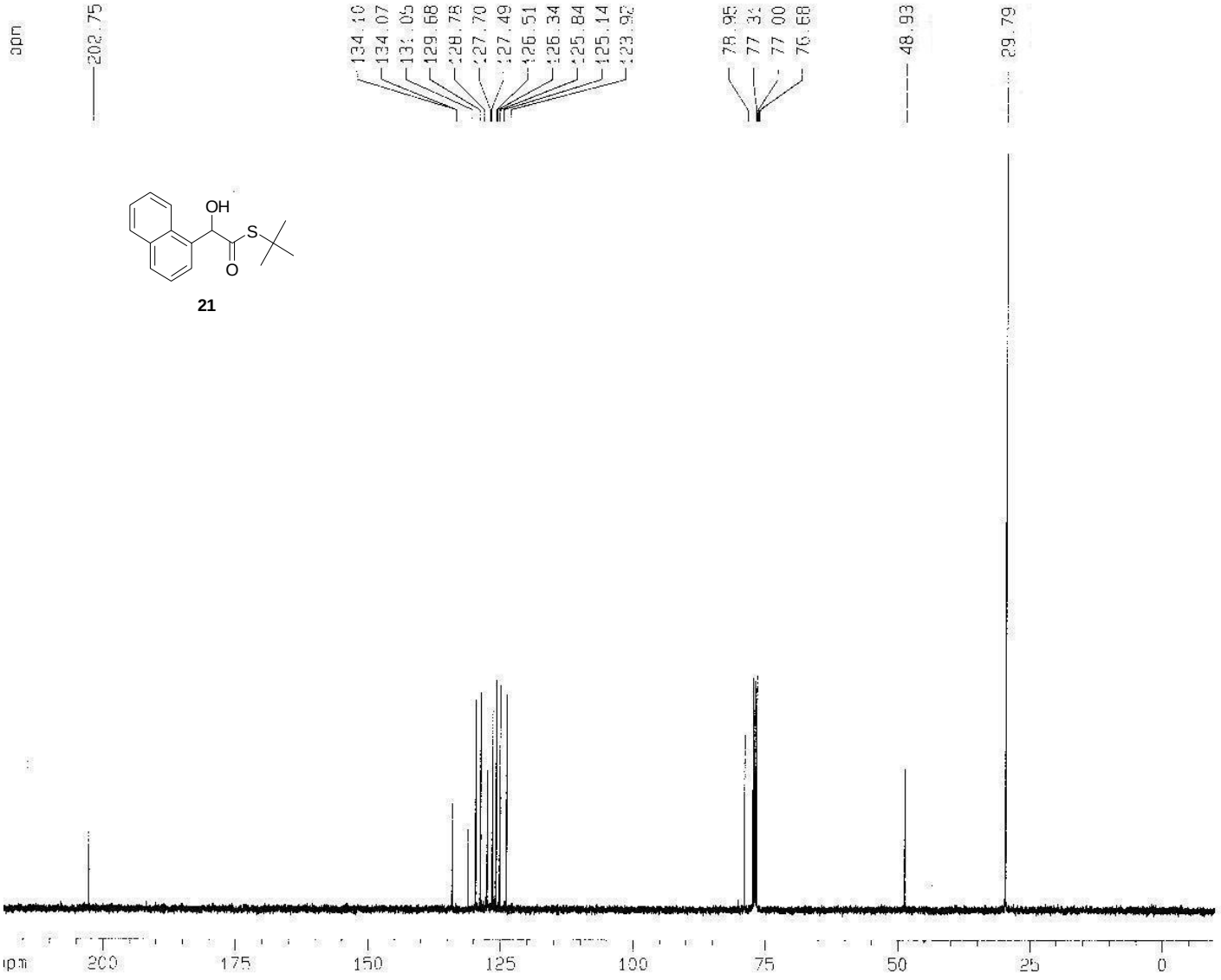

```
NAME        2-OMe-HT-H sam
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20060226
Time               19.52
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                    14
DS                     0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ             1.3664756 sec
RG                   512
DW                83.400 usec
DE                 6.50 usec
TE                300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.10 usec
PL1                3.00 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300095 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 10.50 cm
F1P               10.500 ppm
F1               4201.37 Hz
F2P               -0.500 ppm
F2              -200.07 Hz
PPMCM           0.55000 ppm/cm
HZCM          220.07152 Hz/cm
```



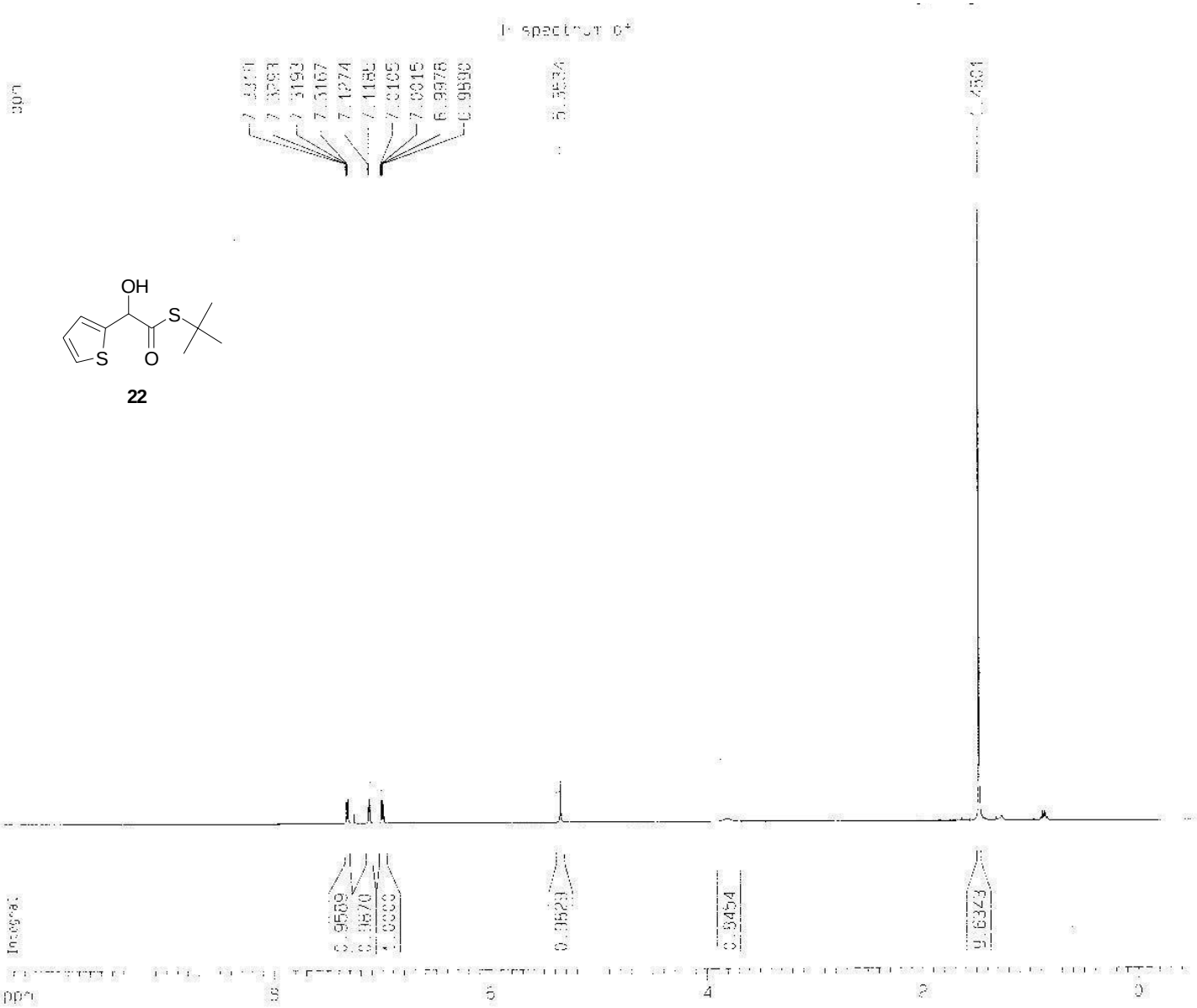

```
Current Data Parameters
NAME          2-OMe-HT C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_          20060226
Time              20 05
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                    68
DS                     0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ            1.3042164 sec
RG                 4096
DW               19.900 usec
DE                6.50 usec
TE               300.0 K
D1           1.20000005 sec
D11          0.03000000 sec
D12          0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                32768
SF          100.6127782 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                11.00 cm
F1P              239.374 ppm
F1               24084.06 Hz
F2P               -10.352 ppm
F2               -1041.57 Hz
PPMCM            12.48630 ppm/cm
HZCM          1256.28149 Hz/cm
```



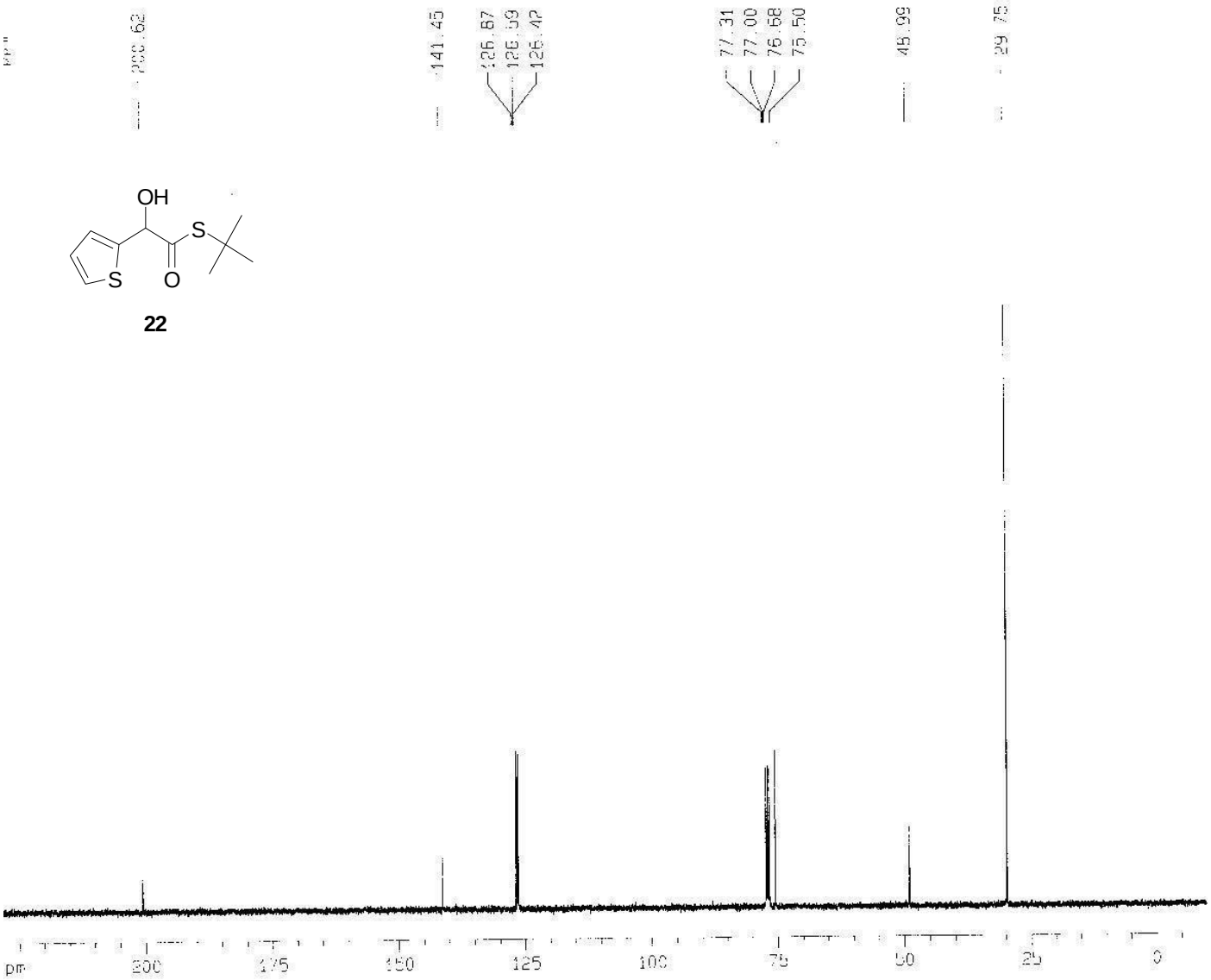

```
NAME                 TH-NaB
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_             20060322
Time                 16.57
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                   16384
SOLVENT              CDCl3
NS                      60
DS                       0
SWH               5995.204 Hz
FIDRES            0.365918 Hz
AQ               1.3664756 sec
RG                     512
DW                  83.400 usec
DE                    6.50 usec
TE                   300.0 K
D1              1.50000000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                    10.10 usec
PL1                    3.00 dB
SFO1           400.1326008 MHz

F2 - Processing parameters
SI                   16384
SF             400.1300099 MHz
WDW                     EM
SSB                      0
LB                    0.10 Hz
GB                       0
PC                    1.00

1D NMR plot parameters
CX                   20.00 cm
CY                   15.00 cm
F1P                 10.500 ppm
F1                 4201.37 Hz
F2P                 -0.500 ppm
F2                -200.07 Hz
PPMCM              0.55000 ppm/cm
HZCM             220.07152 Hz/cm
```



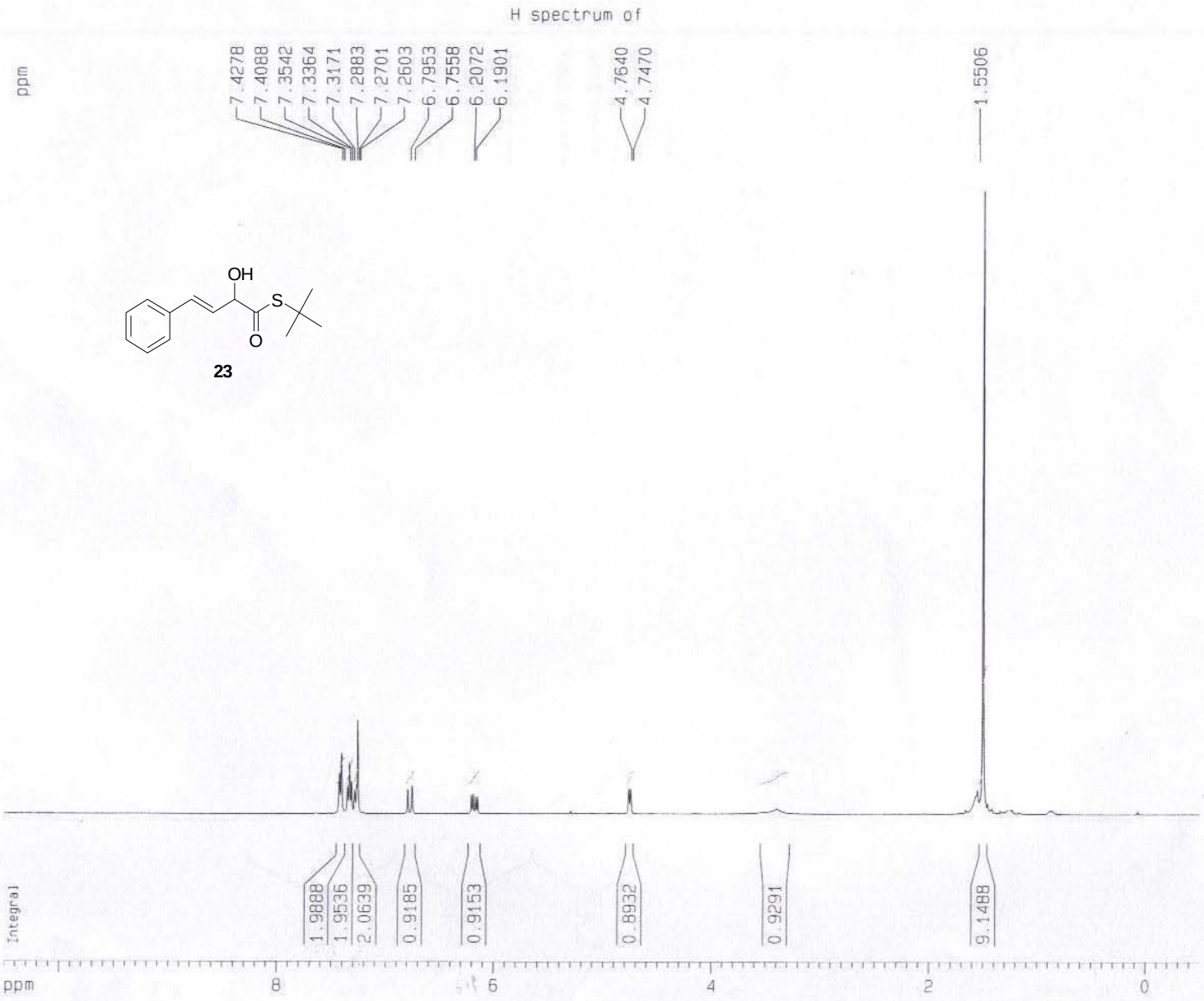

```
Current Data Parameters
NAME          1-Nap-RI-C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_          20060326
Time              16.45
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  140
DS                    0
SWH           25125.629 Hz
FIDRES         0.383397 Hz
AQ            1.3042154 sec
RG                 4096
DW               19.900 usec
DE                6.50 usec
TE               300.0 K
D1            1.20000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.80 usec
PL1                7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.60 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                32768
SF          100.6127782 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                12.50 cm
F1P              220.000 ppm
F1                22134.81 Hz
F2P               -10.000 ppm
F2                1006.13 Hz
PPMCM            11.50000 ppm/cm
HZCM          1157.04700 Hz/cm
```



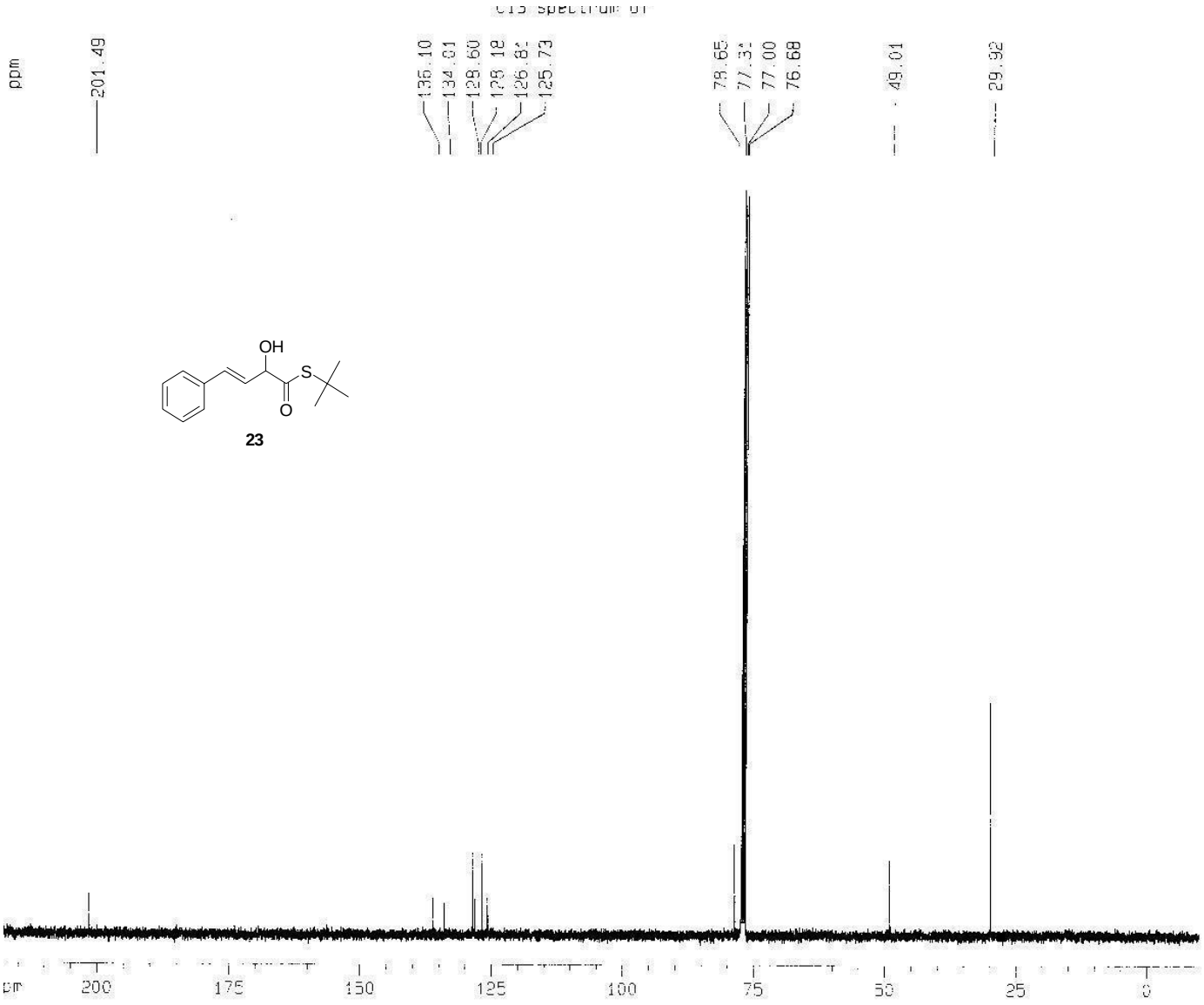

```
NAME      Ben thiophene --
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_          20060416
Time               16.03
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                 16384
SOLVENT            CDCl3
NS                    16
DS                     0
SWH            6896.204 Hz
FIDRES         0.365916 Hz
AQ             2.3664768 sec
RG                  71.6
DW                 84.400 usec
DE                  6.50 usec
TE                 300.0 K
D1             1.00000000 sec

-------- CHANNEL f1 --------
NUC1                   1H
P1                 10.10 usec
PL1                 3.00 dB
SFO1         400.1320005 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.10 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
CY                  10.50 cm
F1P                10.500 ppm
F1                 4201.37 Hz
F2P                -0.500 ppm
F2                -200.06 Hz
PPMCM              0.55000 ppm/cm
HZCM             220.07150 Hz/cm
```



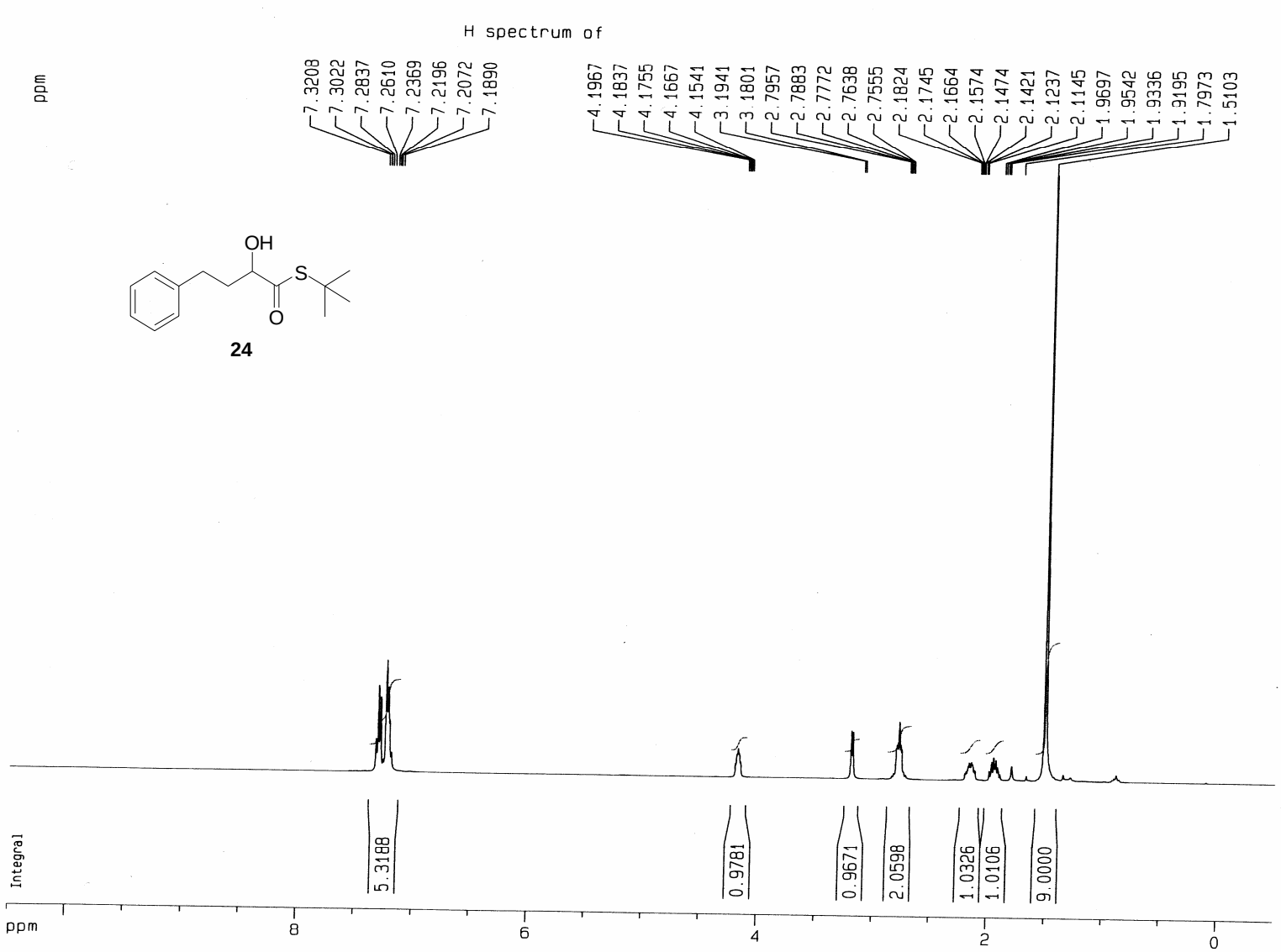

```
Current Data Parameters
NAME      sam thioch-HI H
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20060417
Time                15.40
INSTRUM             spect
PROBHD   5 mm BBO BB-H
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   170
DS                     0
SWH            25125.629 Hz
 IDRES          0.383367 Hz
AQ             1.3042164 sec
RG                  8192
DW                10.000 usec
DE                 6.50 usec
TE                 300.0 K
D1             1.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                  10.80 usec
PL1                  7.00 dB
SFO1          100.6242996 MHz

==== CHANNEL f2 =======
CPDPRG2          waltz16
NUC2                   1H
PCPD2               90.00 usec
PL2                  3.00 dB
PL12                21.83 dB
PL13                24.83 dB
SFO2          400.1319000 MHz

F2 - Processing parameters
SI                   32768
SF            100.5127759 MHz
WDW                     LM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40

1D NMR plot parameters
CX                   20.00 cm
CY                   19.00 cm
F1P                 230.000 ppm
F1                 23140.84 Hz
F2P                 -10.000 ppm
F2                 -1006.13 Hz
PPMCM             12.00000 ppm/cm
HZCM             1207.65337 Hz/cm
```




```
NAME          sam-cinna HT
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_            20060408
Time                18.45
INSTRUM             spect
PROBHD    5 mm BBO BB-1H
PULPROG              zg30
TD                  16384
SOLVENT             CDCl3
NS                     16
DS                      0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ            1.3664756 sec
RG                  406.4
DW                 83.400 usec
DE                   6.50 usec
TE                  300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.10 usec
PL1                  3.00 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                  16384
SF          400.1300088 MHz
WDW                    EM
SSB                     0
LB                   0.10 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
CY                  10.50 cm
F1P                10.500 ppm
F1                4201.37 Hz
F2P                -0.500 ppm
F2                -200.06 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07150 Hz/cm
```

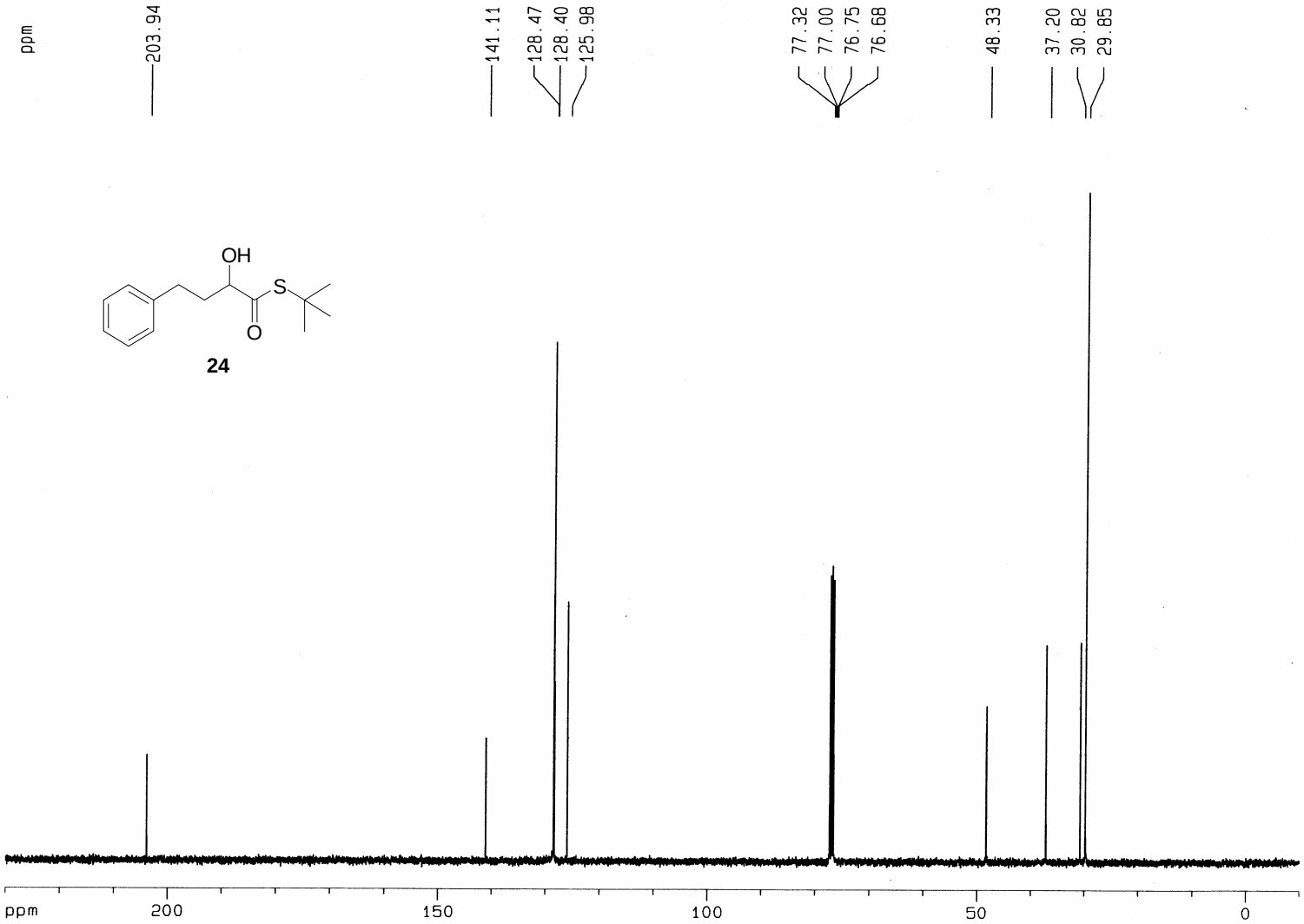



```
Current Data Parameters
NAME        sam-naco.HT-C
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20060408
Time                19.20
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   449
DS                     0
SWH            25125.629 Hz
FIDRES          0.383387 Hz
AQ             1.3042164 sec
RG                  4096
DW                19.900 usec
DE                 6.50 usec
TE                300.0 K
D1             1.20000005 sec
d11            0.03000000 sec
d12            0.00002000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.80 usec
PL1                 7.00 dB
SFO1          100.6242995 MHz

====== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 3.00 dB
PL12               21.83 dB
PL13               24.90 dB
SFO2          400.1319000 MHz

F2 - Processing parameters
SI                  32768
SF            100.6127706 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

13 NMR plot parameters
CX                  20.00 cm
CY                  12.50 cm
F1P                220.000 ppm
F1                 22134.81 Hz
F2P                -10.000 ppm
F2                 1006.13 Hz
PPMCM             11.00000 ppm/cm
HZCM            1107.04688 Hz/cm
```

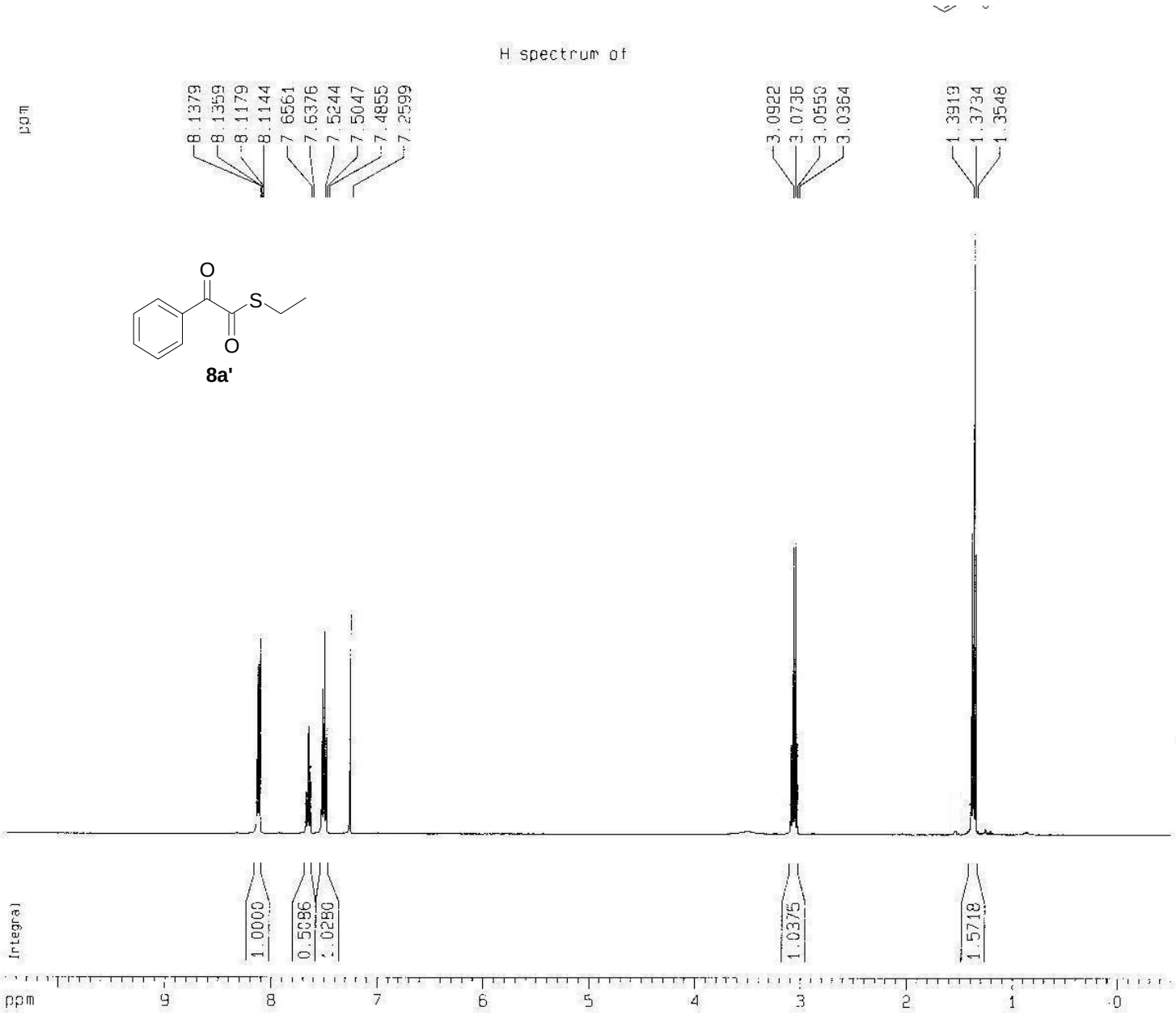



```
Current Data Parameters
NAME                Alph-TH
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_               20060914
Time                   17.38
INSTRUM                spect
PROBHD     5 mm BBO BB-1H
PULPROG                   zg
TD                     16384
SOLVENT                CDCl3
NS                        32
DS                         0
SWH                5995.204 Hz
FIDRES             0.365918 Hz
AQ               1.3664756 sec
RG                     228.1
DW                  83.400 usec
DE                   6.50 usec
TE                   298.6 K
D1              1.50000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     7.50 usec
PL1                   23.00 dB
SFO1            400.1326008 MHz

F2 - Processing parameters
SI                     16384
SF              400.1300088 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     20.00 cm
CY                     15.00 cm
F1P                   10.500 ppm
F1                   4201.37 Hz
F2P                   -0.500 ppm
F2                   -200.06 Hz
PPMCM               0.55000 ppm/cm
HZCM              220.07150 Hz/cm
```

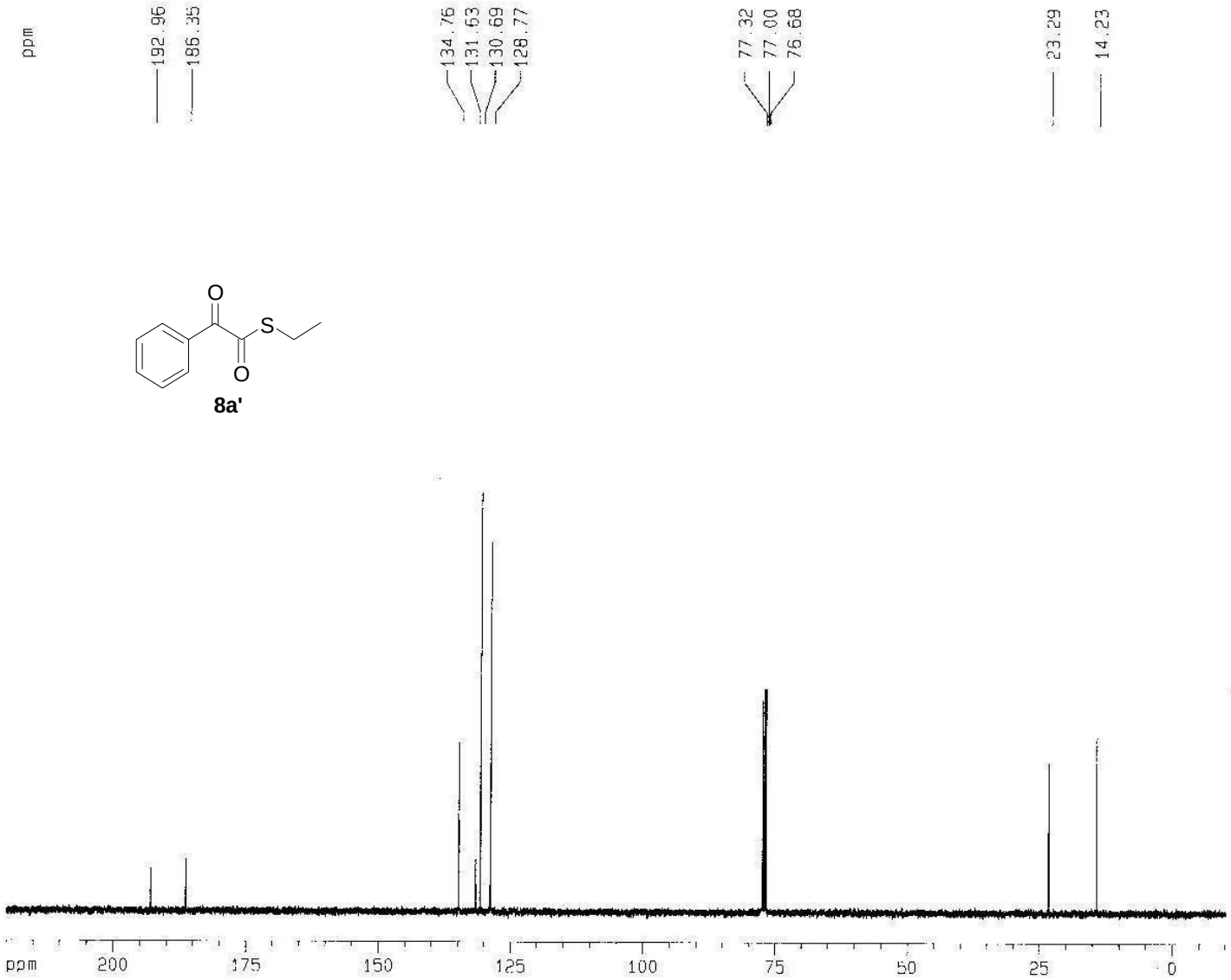
C13 spectrum of



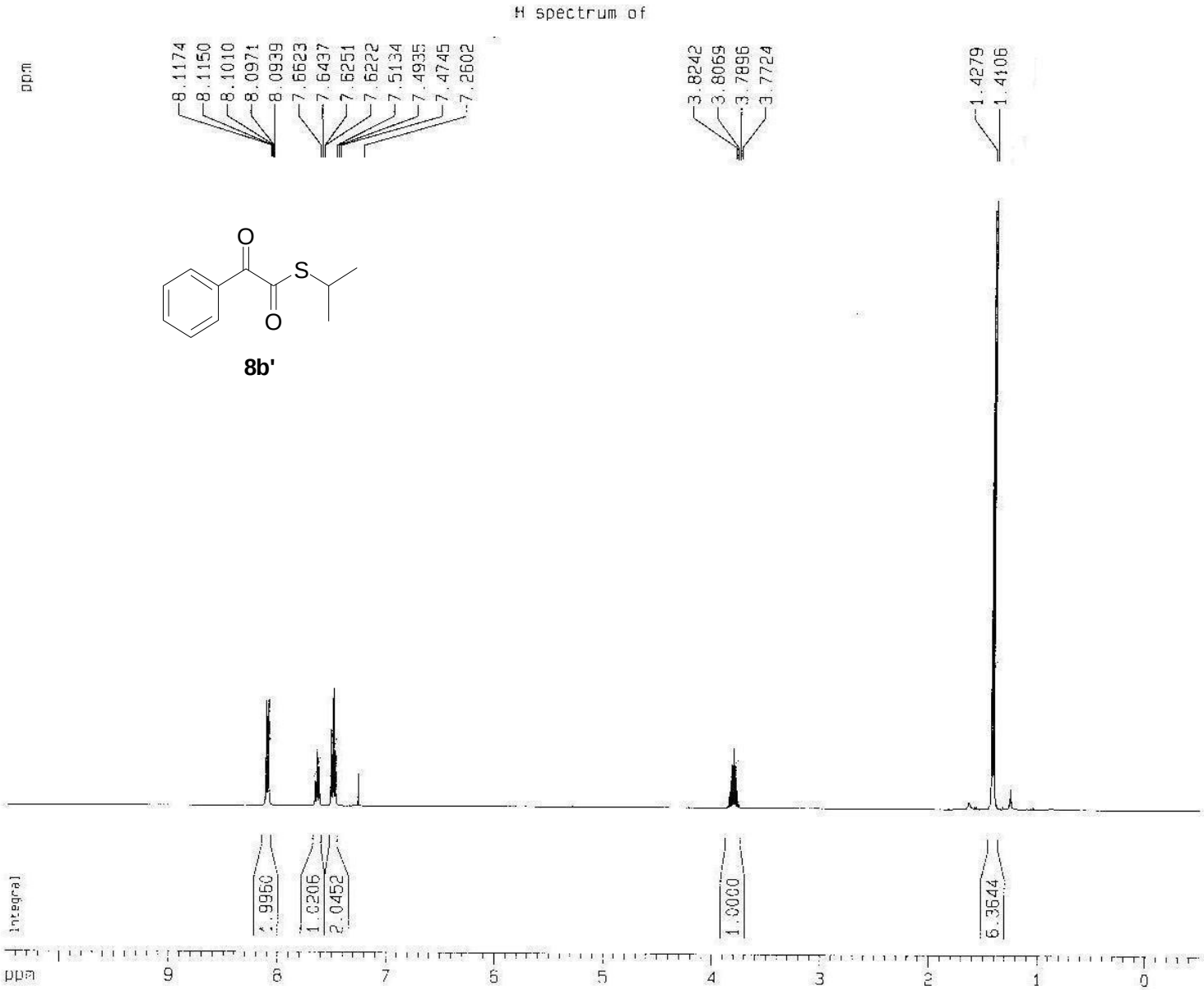

```
Current Data Parameters
NAME              Alph-TH
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20060914
Time               17.44
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  118
DS                    0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ            1.3042164 sec
RG                 8192
DW               19.900 usec
DE                6.50 usec
TE                298.7 K
D1           1.20000005 sec
d11          0.03000000 sec
DELTA        1.10000002 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1               10.80 usec
PL1               7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2               3.00 dB
PL12             21.83 dB
PL13             24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                32768
SF          100.6127782 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                12.50 cm
F1P              230.000 ppm
F1             23140.94 Hz
F2P             -10.000 ppm
F2             -1006.13 Hz
PPMCM          12.00000 ppm/cm
HZCM         1207.35327 Hz/cm
```




```
Current Data Parameters
NAME      ethane thio ket
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date            20051021
Time               20.09
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ            1.3664756 sec
RG                 406.4
DW                83.400 usec
DE                  6.50 usec
TE                 300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.10 usec
PL1                 3.00 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300095 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 10.50 cm
F1P                10.500 ppm
F1               4201.37 Hz
F2P                -0.500 ppm
F2               -200.07 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07152 Hz/cm
```

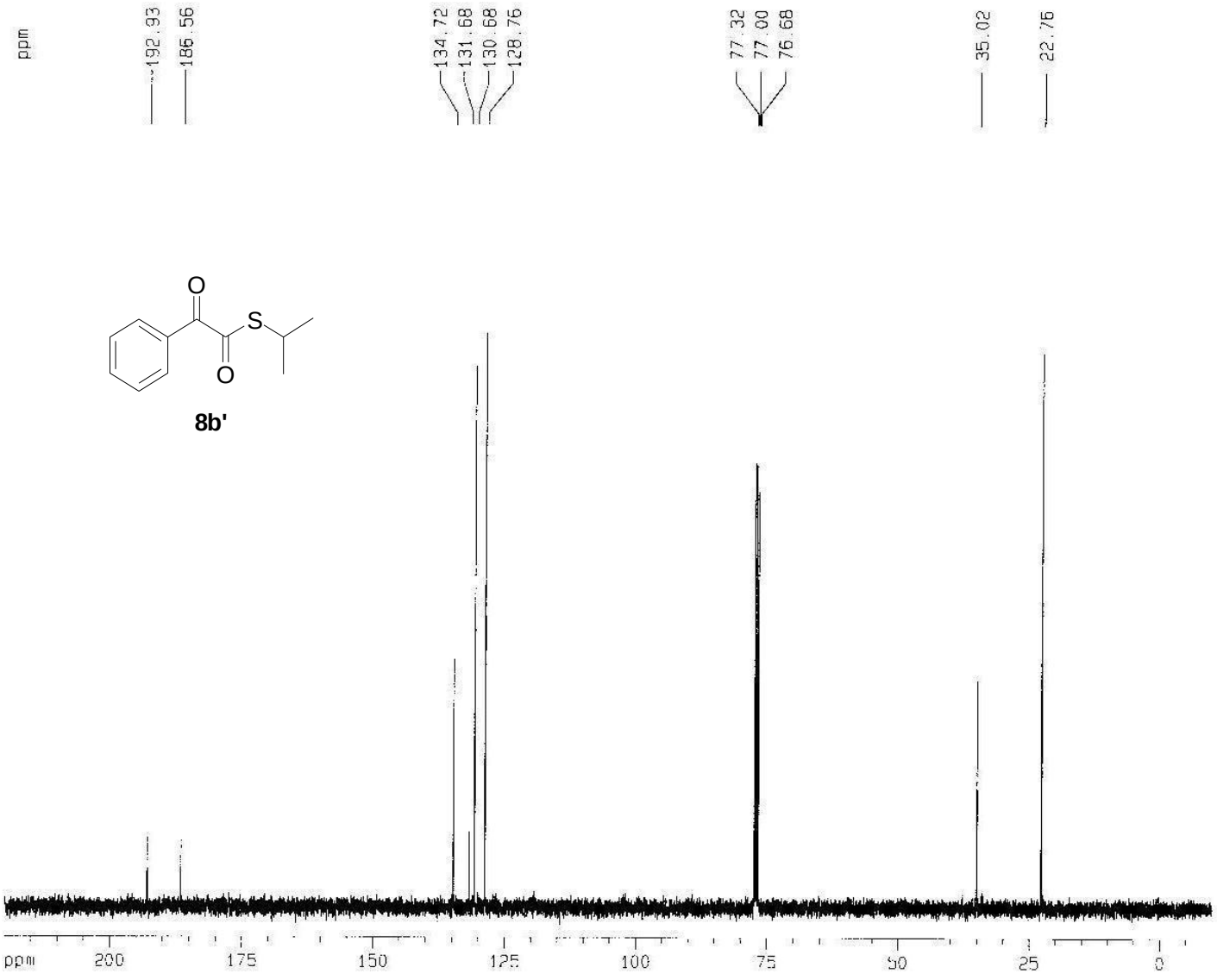



```
Current Data Parameters
NAME          thioketone
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20051027
Time              13.29
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  146
DS                    0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ            1.3042164 sec
RG                 8192
DW               19.900 usec
DE                6.50 usec
TE               300.0 K
D1            1.20000005 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                10.80 usec
PL1                7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                32768
SF          100.6127744 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                 7.00 cm
F1P             220.000 ppm
F1              22134.81 Hz
F2P              -10.314 ppm
F2              -1037.74 Hz
PPMCM           11.51571 ppm/cm
HZCM          1158.62769 Hz/cm
```



8b'

```
NAME        sam-iso-HT-Ket-1
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_             20060528
Time                 16.23
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG              zg30
TD                  16384
SOLVENT             CDCl3
NS                     16
DS                      0
SWH              5995.204 Hz
FIDRES           0.365918 Hz
AQ              1.3664756 sec
RG                    114
DW                 83.400 usec
DE                  6.50 usec
TE                 300.0 K
D1              1.50000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.10 usec
PL1                  3.00 dB
SFO1           400.1325008 MHz

F2 - Processing parameters
SI                  16384
SF            400.1300091 MHz
WDW                    EM
SSB                     0
LB                   0.10 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
CY                  10.50 cm
F1P                10.500 ppm
F1               4201.37 Hz
F2P                 0.500 ppm
F2                -200.07 Hz
PPMCM             0.55000 ppm/cm
HZCM            220.07152 Hz/cm
```



Current Data Parameters
NAME sam-iso-HT-Ket-1
EXPNO 2
PROCNO 1

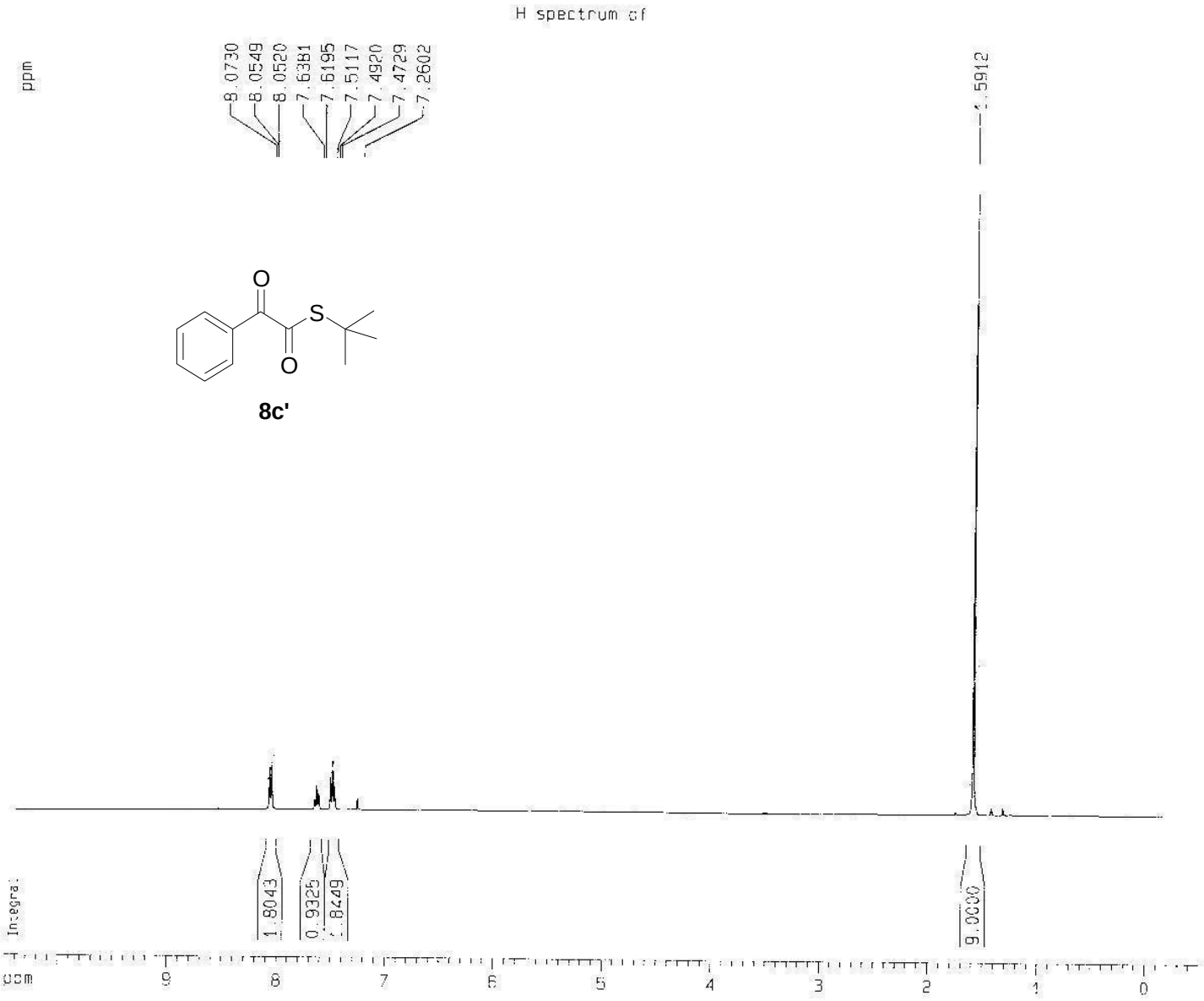
F2 - Acquisition Parameters
Date_ 20060528
Time 16.27
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 102
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 8192
DW 19.900 usec
DE 6.50 usec
TE 300.0 K
D1 1.20000005 sec
d11 0.03000000 sec
d12 0.00002000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 10.80 usec
PL1 7.00 dB
SFO1 100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 21.83 dB
PL13 24.80 dB
SFO2 400.1319000 MHz

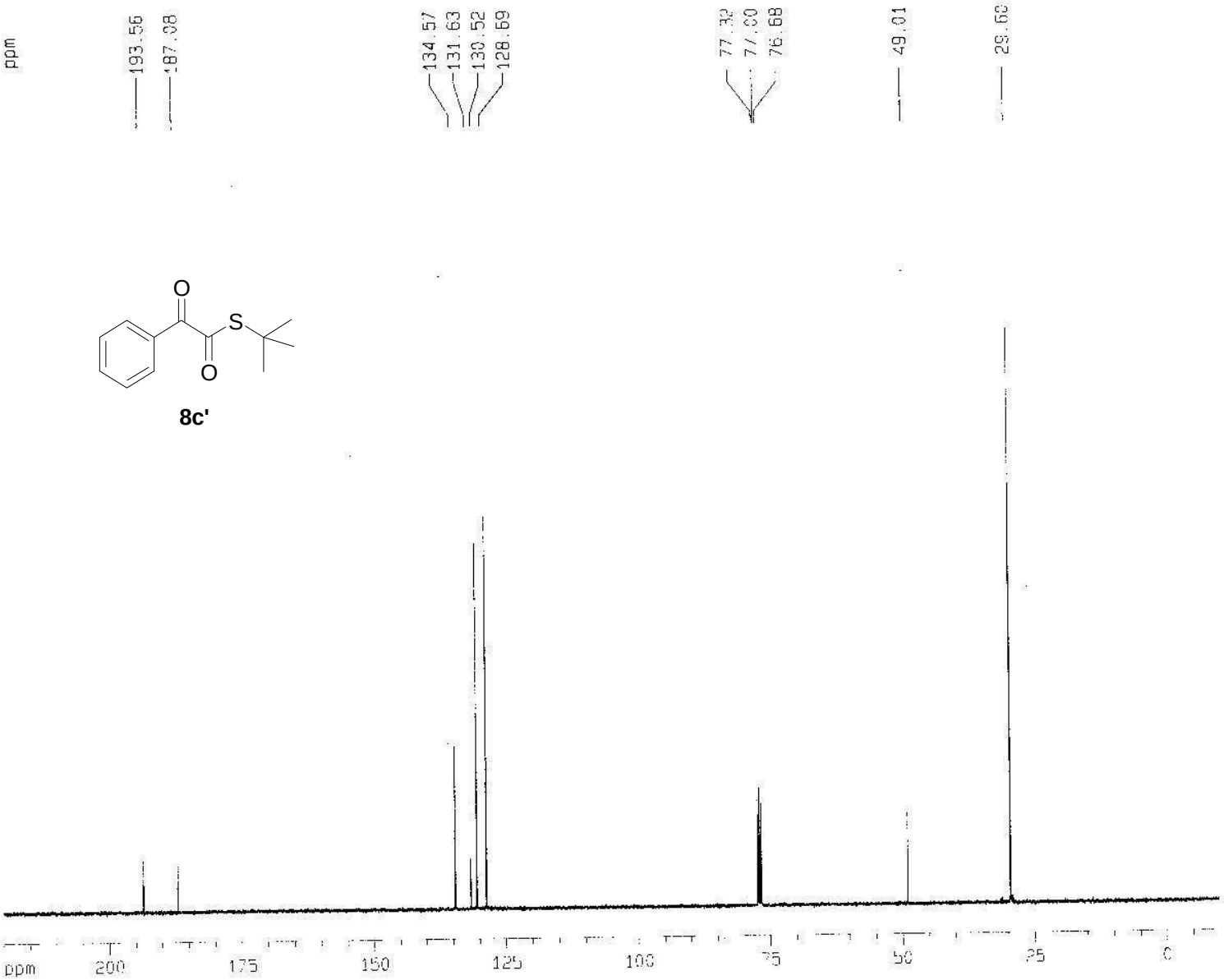
F2 - Processing parameters
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 220.000 ppm
F1 22134.61 Hz
F2P -10.000 ppm
F2 -1006.13 Hz
PPMCM 11.50000 ppm/cm
HZCM 1157.04698 Hz/cm

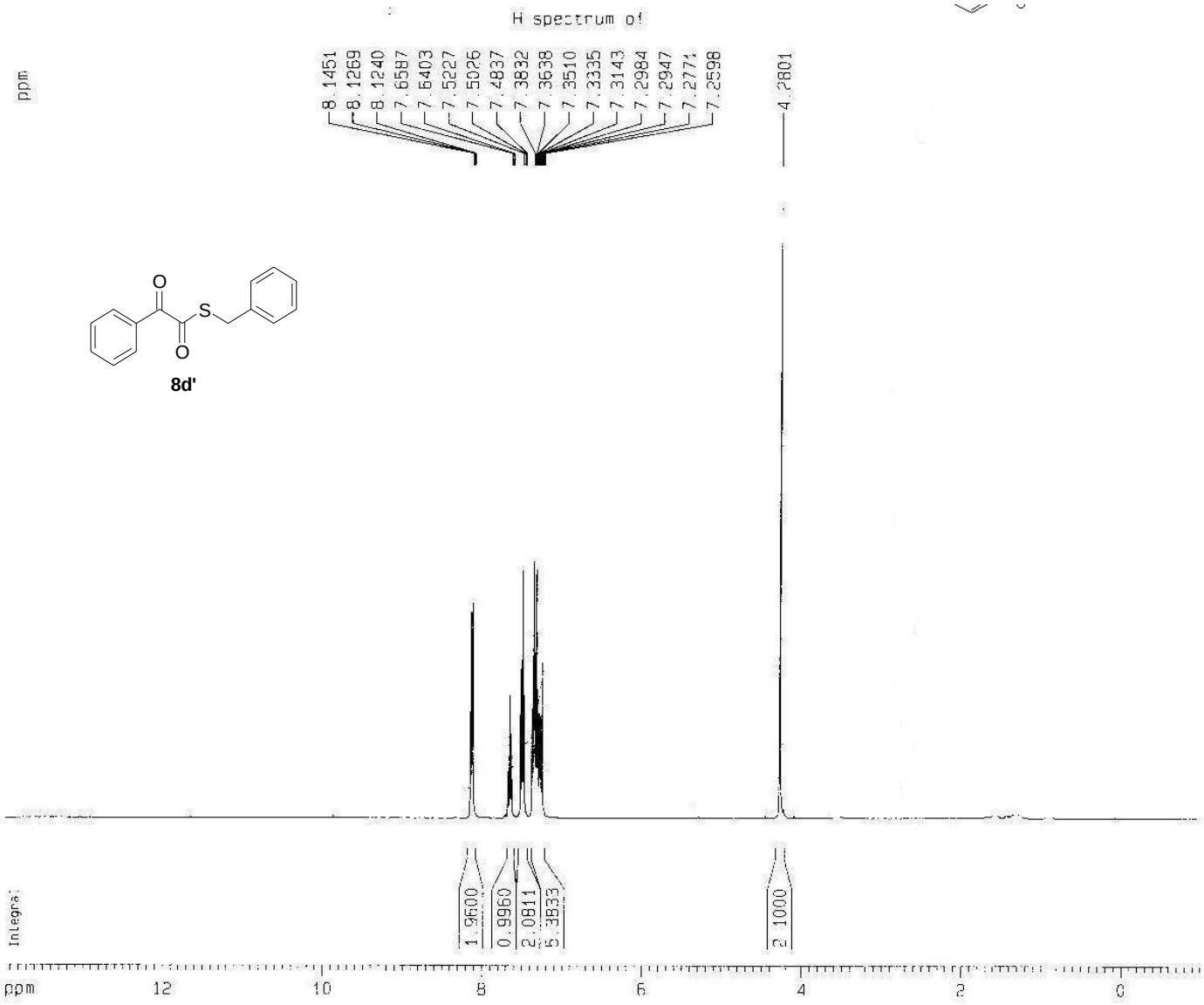



```
Current Data Parameters
NAME      sam-phenyl-HT-KI-H
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_           20060528
Time               14 35
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                16384
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            5995.204 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                  114
DW               83.400 usec
DE                6.50 usec
TE               300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.10 usec
PL1                3.00 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300091 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 10.50 cm
F1P               10.500 ppm
F1                4201.37 Hz
F2P                0.500 ppm
F2                -200.07 Hz
PPMCM             0.55000 ppm/cm
HZCM            220.07152 Hz/cm
```

8c'

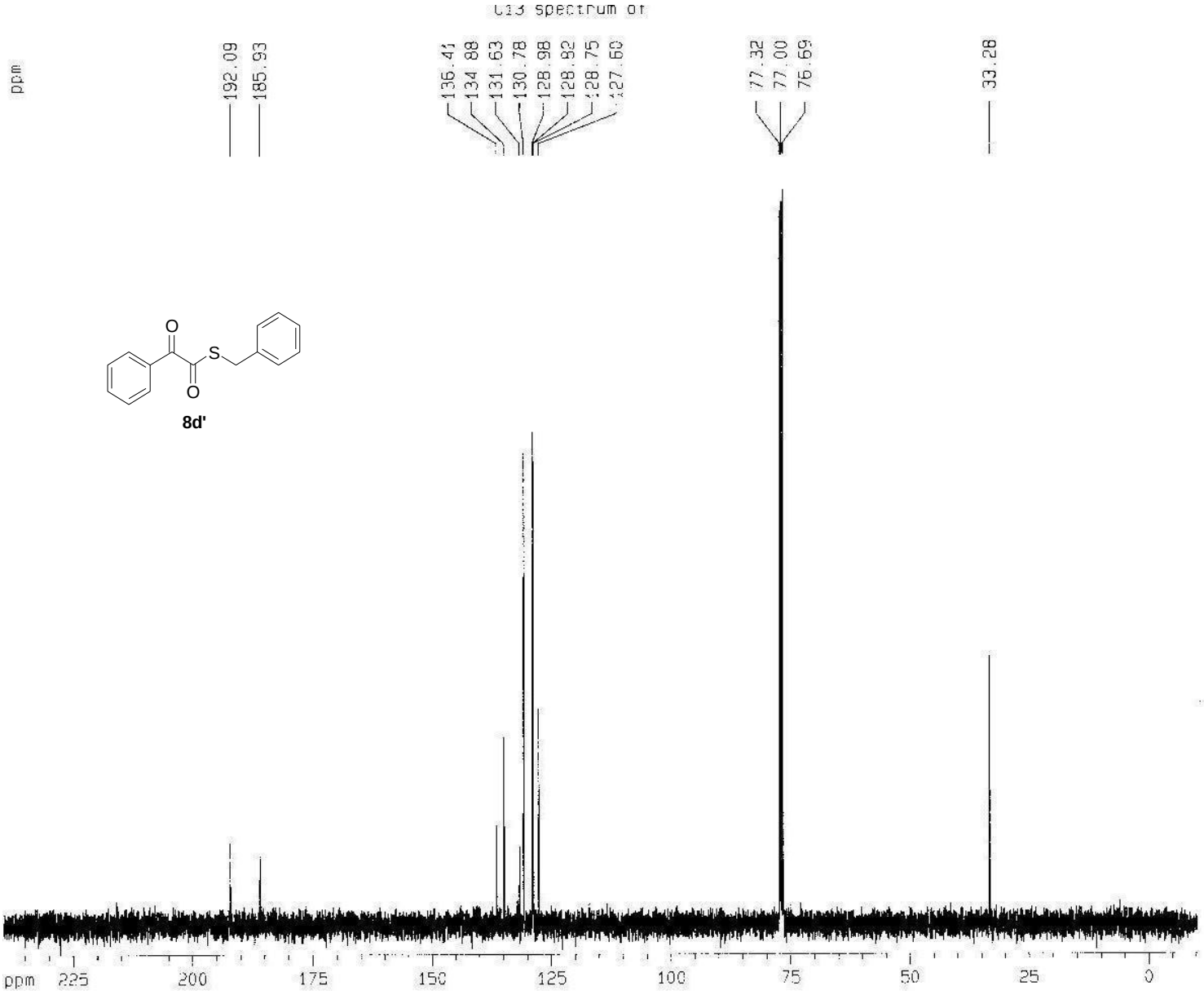



```
Current Data Parameters
NAME            torthio
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20051012
Time              12.37
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD               65536
SOLVENT           CDCl3
NS                  117
DS                    0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ            1.3042154 sec
RG                 4096
DW               19.900 usec
DE                6.50 usec
TE               300.0 K
D1            1.20000005 sec
D11           0.03000000 sec
D12           0.00002000 sec

======== CHANNEL f1 =======
NUC1                13C
P1                10.80 usec
PL1               7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 =======
CPDPRG2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               3.00 dB
PL12             21.93 dB
PL13             24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                32768
SF          100.6127775 MHz
WDW                  EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                20.00 cm
F1P             220.000 ppm
F1            22134.81 Hz
F2P             -10.000 ppm
F2            -1006.13 Hz
PPMCM           12.50000 ppm/cm
HZCM          1157.04698 Hz/cm
```



8d'

```
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20060528
Time              14 15
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG           zg30
TD                16384
SOLVENT           CDCl3
NS                  16
DS                   0
SWH            5995.204 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                203.2
DW                83.400 usec
DE                 6.50 usec
TE                300.0 K
D1           1.50000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.10 usec
PL1                3.00 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300095 MHz
WDW                  EM
SSB                   0
LB                 0.10 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                10.50 cm
F1P               13.968 ppm
F1               5588.95 Hz
F2P                1.015 ppm
F2               -406.25 Hz
PPMCM            0.74916 ppm/cm
HZCM           299.76019 Hz/cm
```



Current Data Parameters
NAME sam -S-benzyl-Ket-HT
EXPNO 2
PROCNO 1

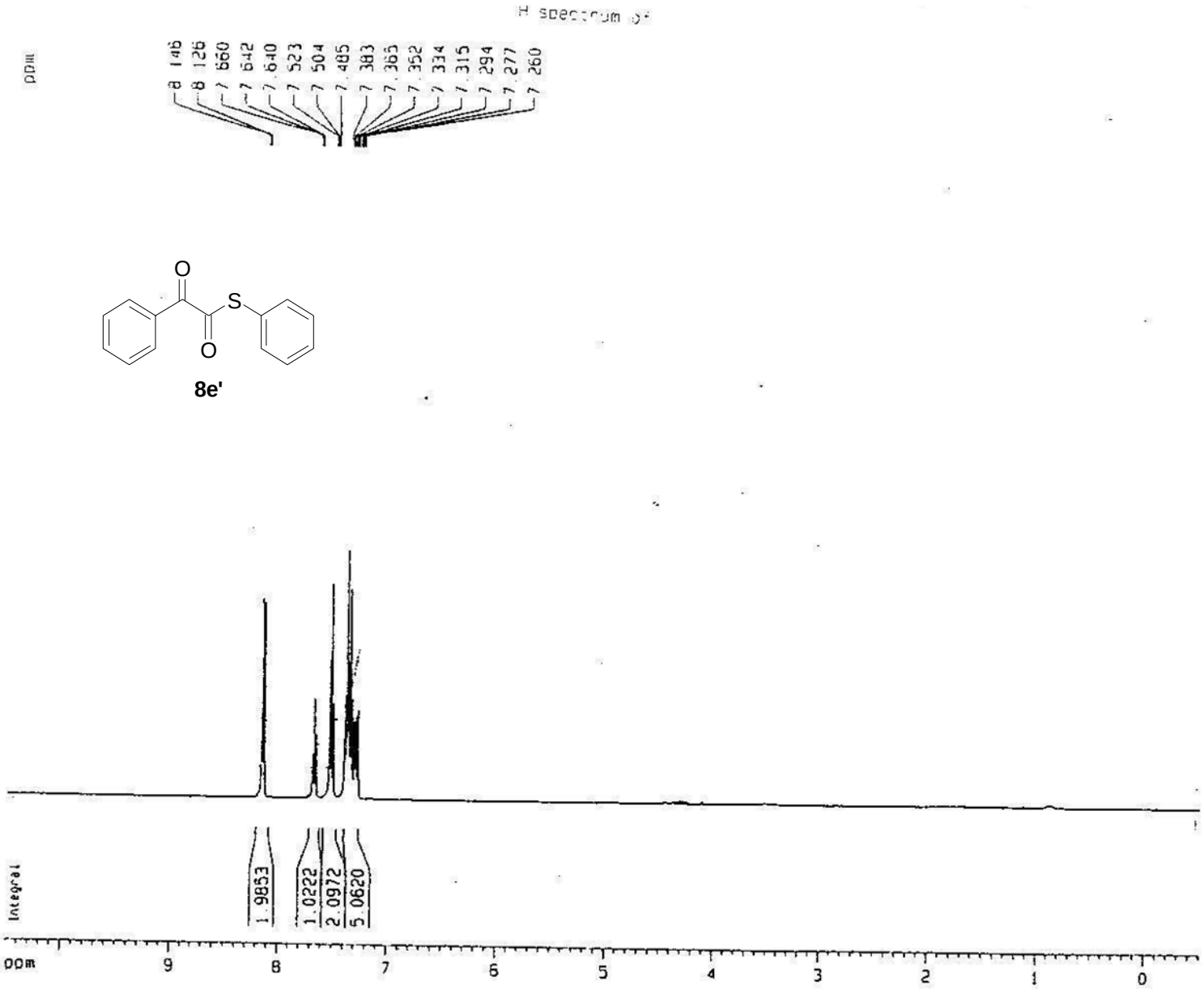
F2 - Acquisition Parameters
Date 20060528
Time 14.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 141
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 4096
DW 19.900 usec
DE 6.50 usec
TE 300.0 K
D1 1.20000005 sec
d11 0.03000000 sec
d12 0.00002000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 10.80 usec
PL1 7.00 dB
SFO1 100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 21.83 dB
PL13 24.80 dB
SFO2 400.1319000 MHz

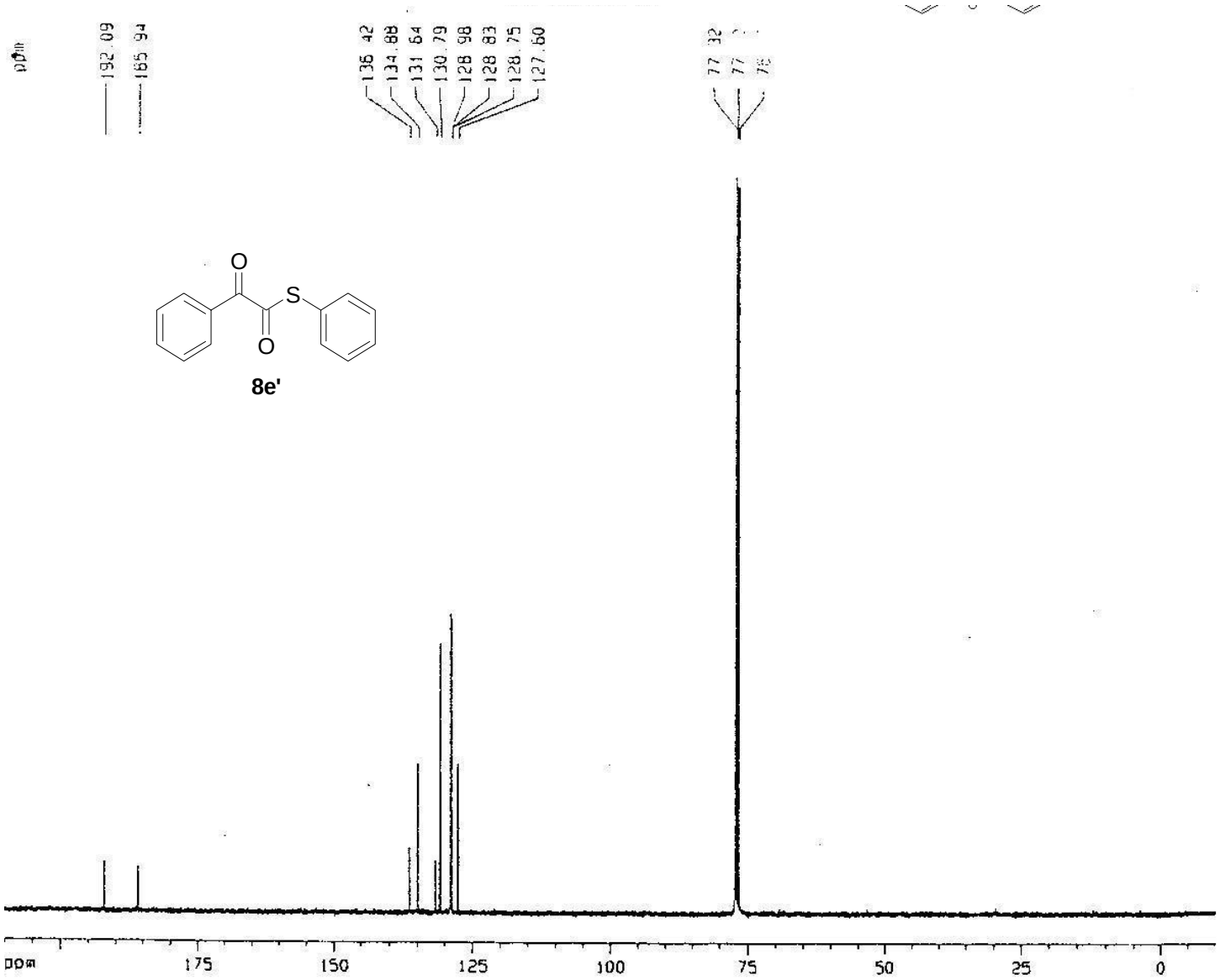
F2 - Processing parameters
SI 32768
SF 100.6127721 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 239.435 ppm
F1 24090.19 Hz
F2P -10.291 ppm
F2 -1035.44 Hz
PPMCM 12.48630 ppm/cm
HZCM 1256.28137 Hz/cm

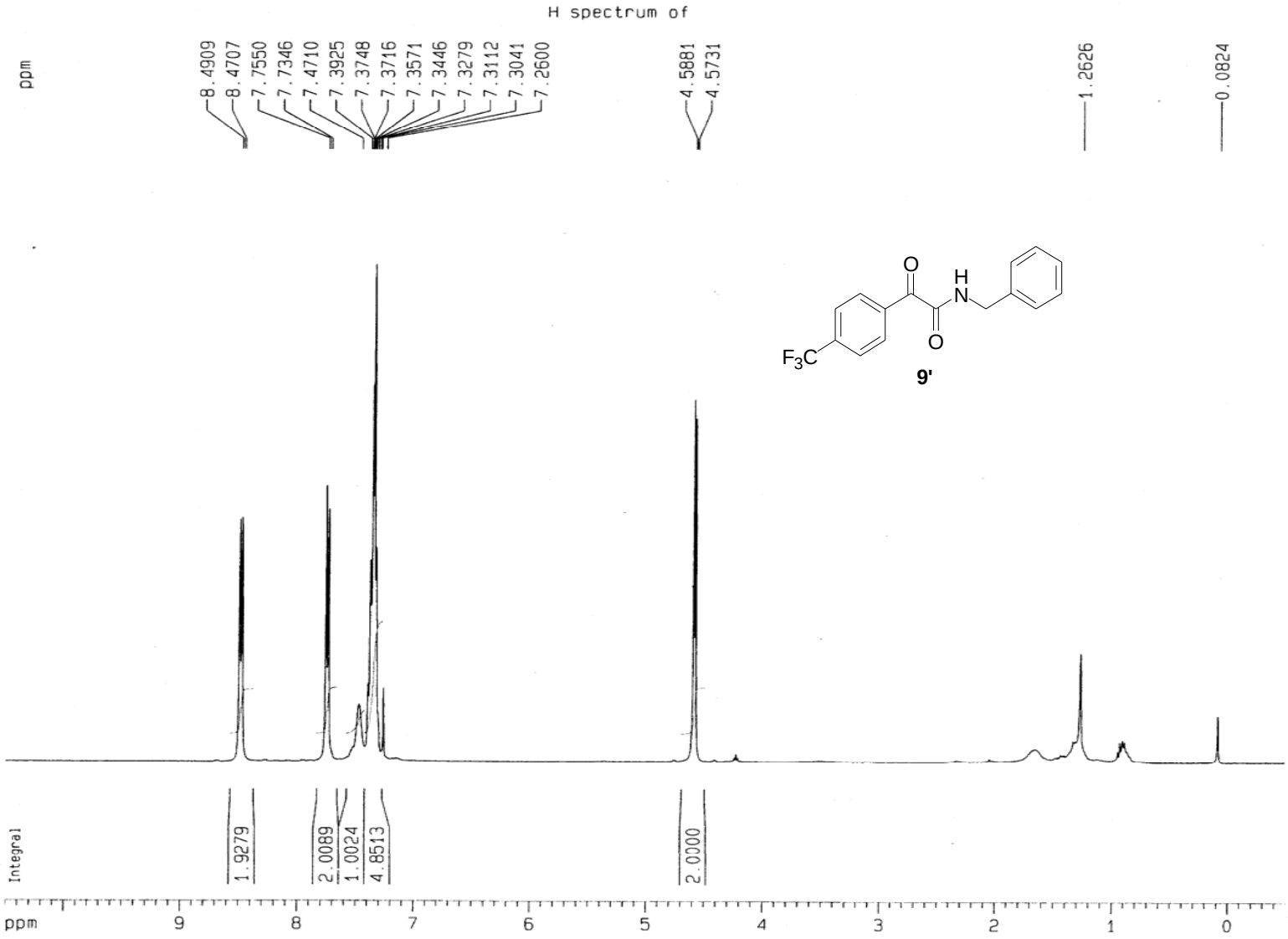


8e'

```
NAME          2-exp
EXPNO             2
PROCNO            1

F2 - Acquisition Parameters
Date_        2006-519
Time            19 53
INSTRUM         spect
PROBHD   5 mm BBO BB-1H
PULPROG         zg30
TD             16384
SOLVENT        CDCl3
NS                16
DS                 0
SWH         5995.204 Hz
FIDRES      0.365918 Hz
AQ          1.3664756 sec
RG             22.6
DW            83.400 us
DE             6.50 us
TE            300.0 K
D1         1.50000000 sec

======== CHANNEL f1 ======
NUC1              1H
P1             10.10 us
PL1             3.00 dB
SFO1      400.1326008 MHz

F2 - Processing parameters
SI             16384
SF        400.1300095 MHz
WDW               EM
SSB                0
LB              0.10 Hz
GB                 0
PC             1.00

1D NMR plot parameters
CX             20.00 cm
CY              9.00 cm
F1P            10.500 ppm
F1            4201.37 Hz
F2P            -0.500 ppm
F2            -200.07 Hz
PPMCM         0.55000 ppm/cm
HZCM         220.07152 Hz/cm
```



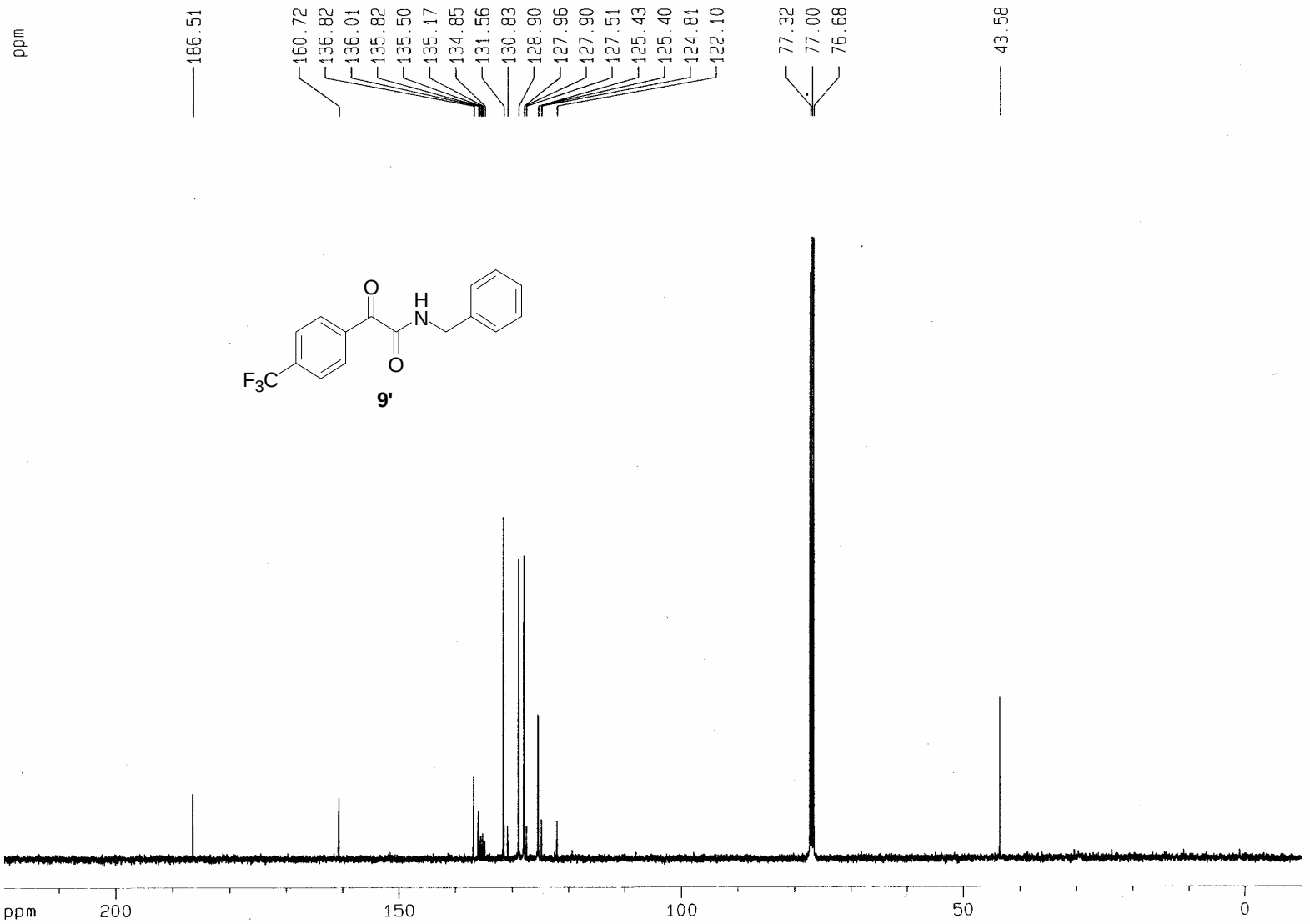

```
Current Data Parameters
NAME          2-exo-069'
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20060519
Time               19.54
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1640
DS                    0
SWH           25125.629 Hz
FIDRES        0.383387 Hz
AQ            1.3042164 sec
RG                 4096
DW               19.900 usec
DE                6.50 usec
TE               300.0 K
D1            1.20000005 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.80 usec
PL1                7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                32768
SF          100.6127713 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                12.50 cm
F1P              210.000 ppm
F1             21128.68 Hz
F2P              -10.000 ppm
F2             -1006.13 Hz
PPMCM           11.00000 ppm/cm
HZCM          1106.74048 Hz/cm
```



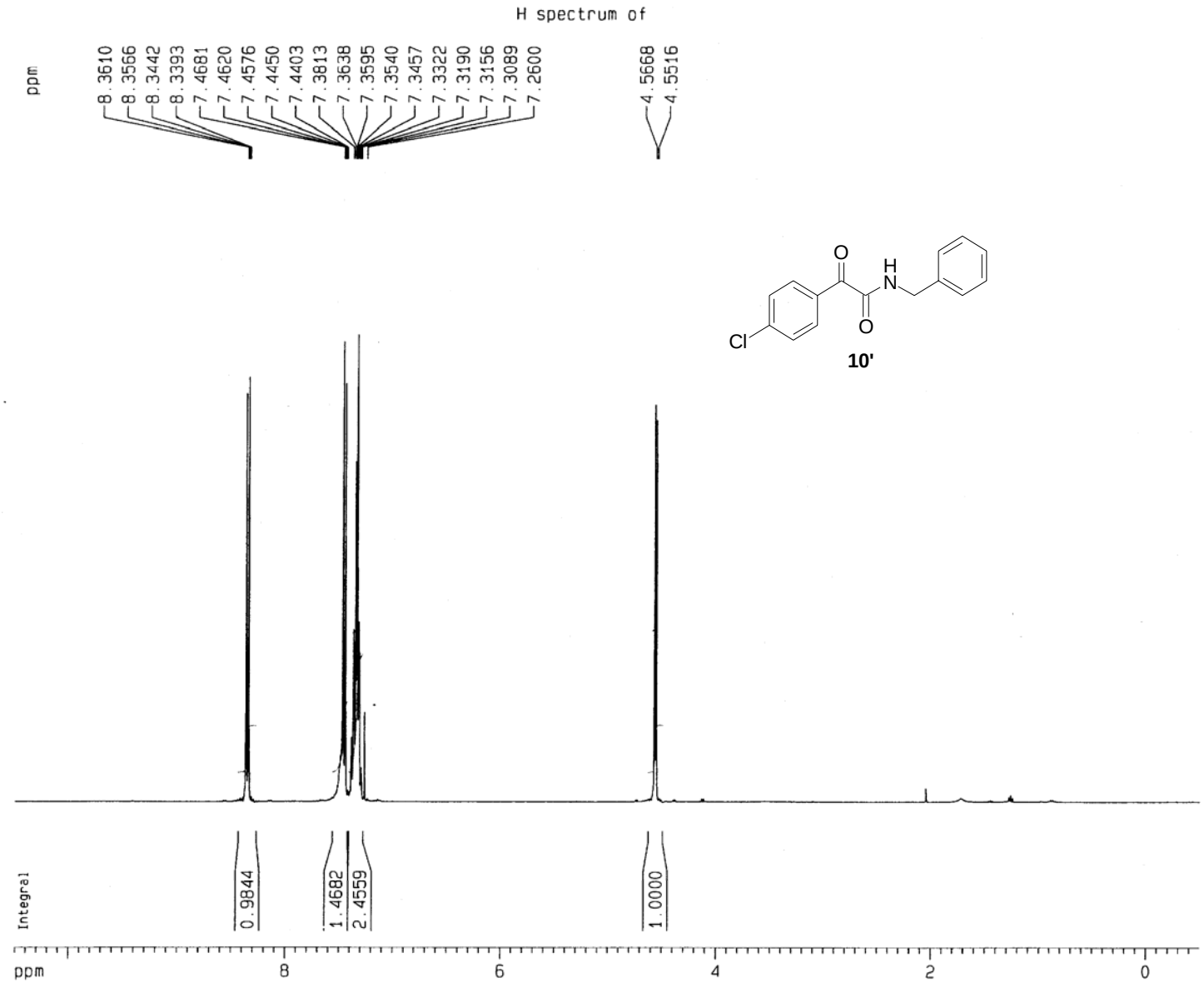
9'

```
Current Data Parameters
NAME          CF3medalate
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20051213
Time               12.46
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                    25
DS                     0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ             1.3664756 sec
RG                   181
DW                83.400 usec
DE                 6.50 usec
TE                300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.10 usec
PL1                3.00 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300099 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                  9.00 cm
F1P               10.500 ppm
F1               4201.37 Hz
F2P               -0.500 ppm
F2               -200.07 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07152 Hz/cm
```

C13 spectrum of



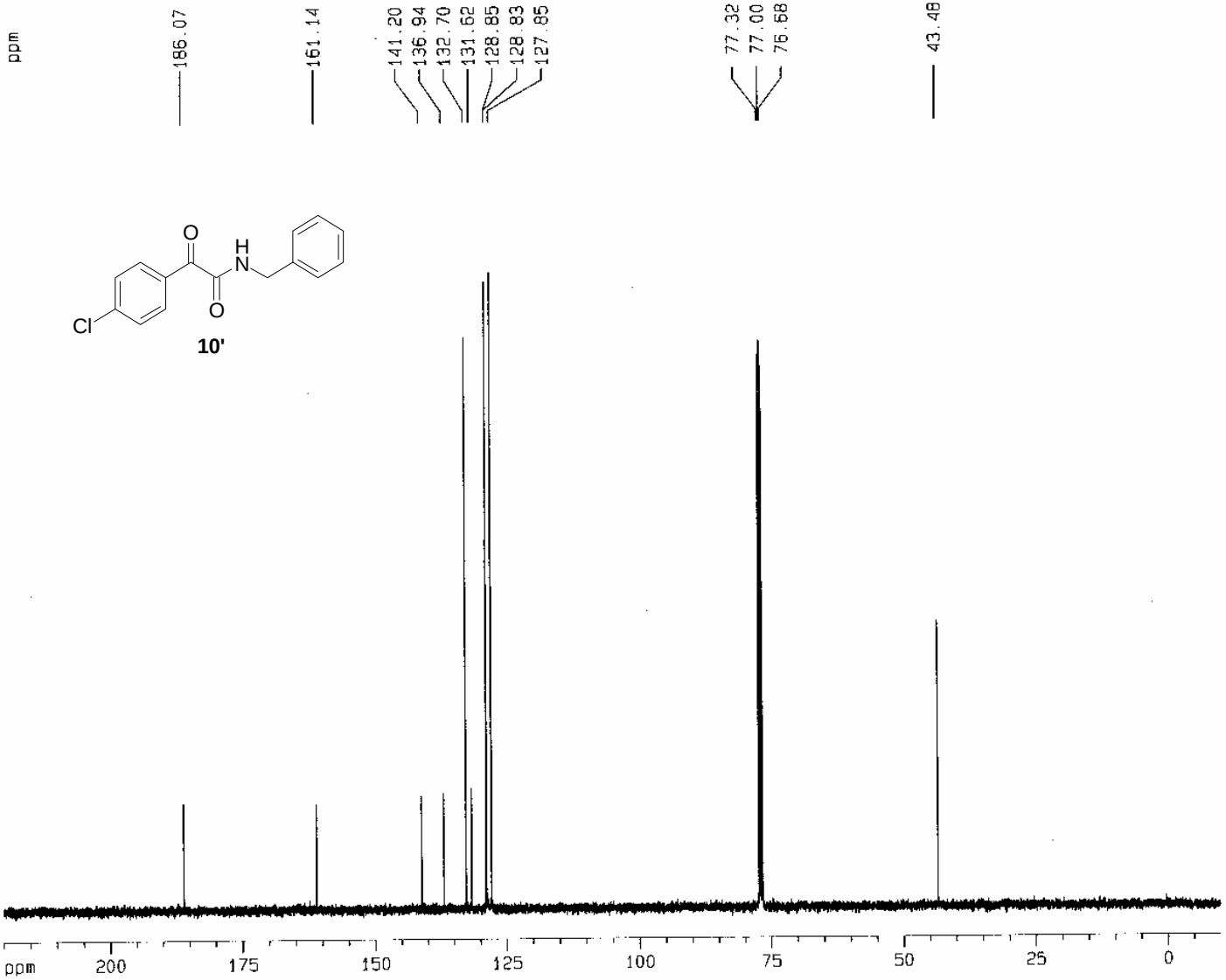

```
Current Data Parameters
NAME          CF3medalate
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_            20051213
Time               12.53
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  824
DS                    0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ            1.3042164 sec
RG                 4096
DW               19.900 usec
DE                6.50 usec
TE                300.0 K
D1           1.20000005 sec
d11          0.03000000 sec
d12          0.00002000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                10.80 usec
PL1                7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2            90.00 usec
PL2               3.00 dB
PL12             21.83 dB
PL13             24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                32768
SF          100.6127729 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                11.00 cm
F1P             220.000 ppm
F1             22134.81 Hz
F2P             -10.000 ppm
F2             -1006.13 Hz
```



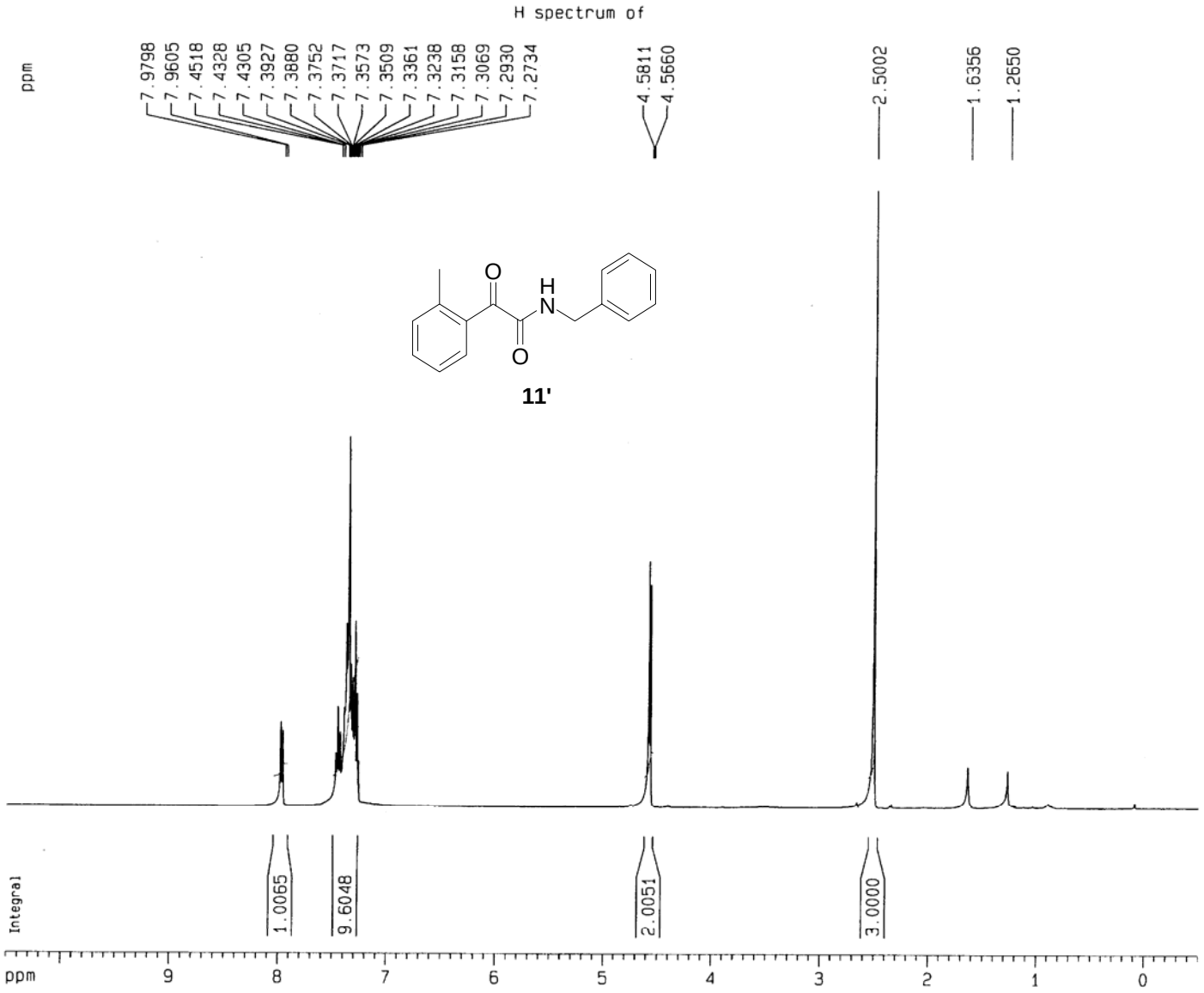
10'

```
Current Data Parameters
NAME      4ClmedelicBnamide
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_            20050304
Time                16.48
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  16384
SOLVENT             CDCl3
NS                      4
DS                      0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ             1.3664756 sec
RG                   22.6
DW                83.400 usec
DE                 6.50 usec
TE                300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.10 usec
PL1                 3.00 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                  16384
SF           400.1300088 MHz
WDW                    EM
SSB                     0
LB                   0.10 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
CY                   8.00 cm
F1P                10.500 ppm
F1                4201.37 Hz
F2P                -0.500 ppm
F2               -200.06 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07150 Hz/cm
```

C13 spectrum of

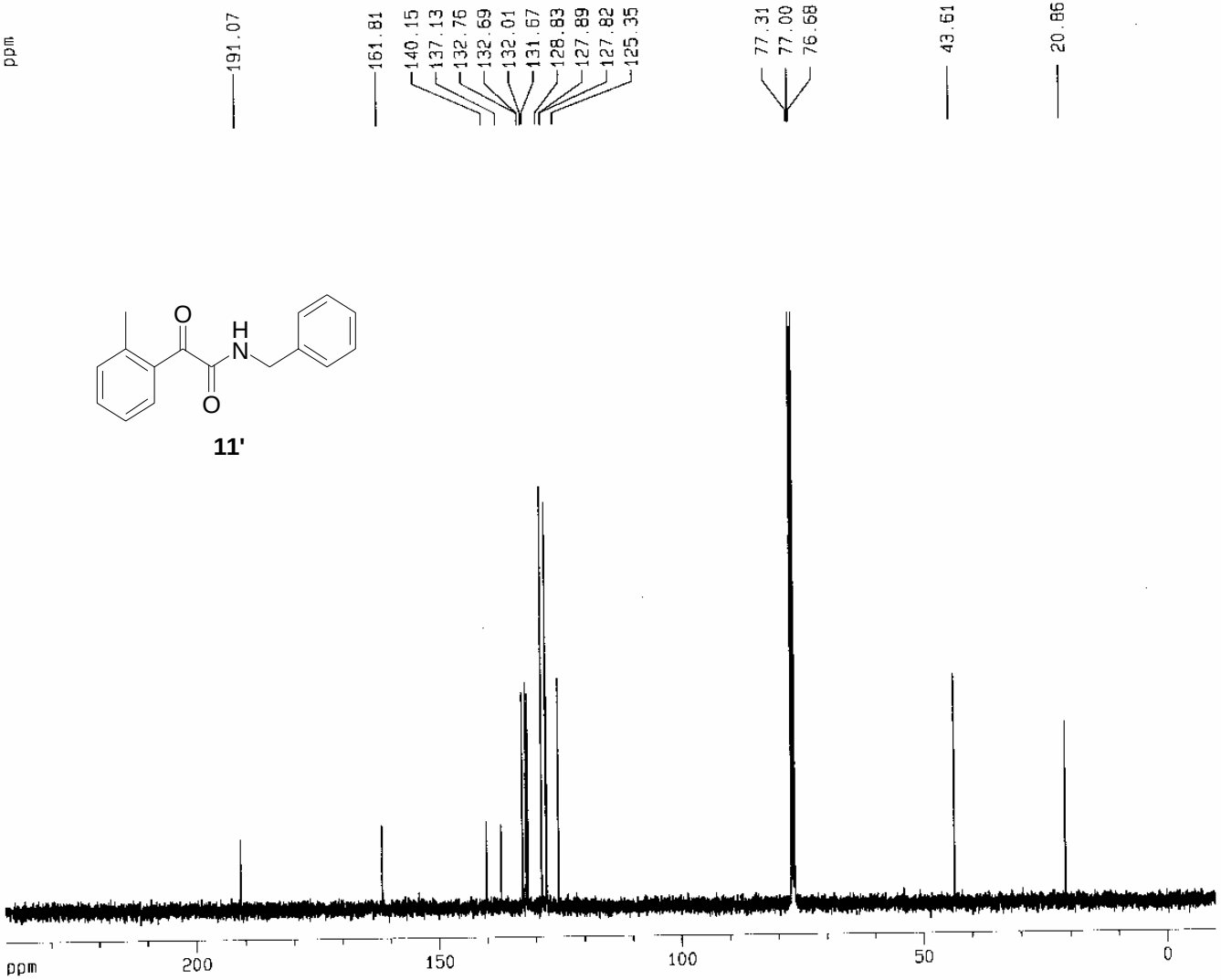



```
Current Data Parameters
NAME      4ClmedelicBnamide
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_            20050304
Time                16.51
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   256
DS                     0
SWH            25125.629 Hz
FIDRES          0.383387 Hz
AQ             1.3042164 sec
RG                  4096
DW                19.900 usec
DE                 6.50 usec
TE                300.0 K
D1             1.20000005 sec
d11            0.03000000 sec
d12            0.00002000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.80 usec
PL1                 7.00 dB
SFO1         100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 3.00 dB
PL12               21.83 dB
PL13               24.80 dB
SFO2         400.1319000 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127752 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 11.00 cm
F1P               220.000 ppm
F1              22134.81 Hz
F2P               -10.000 ppm
F2              -1006.13 Hz
PPMCM            11.50000 ppm/cm
HZCM           1157.04688 Hz/cm
```



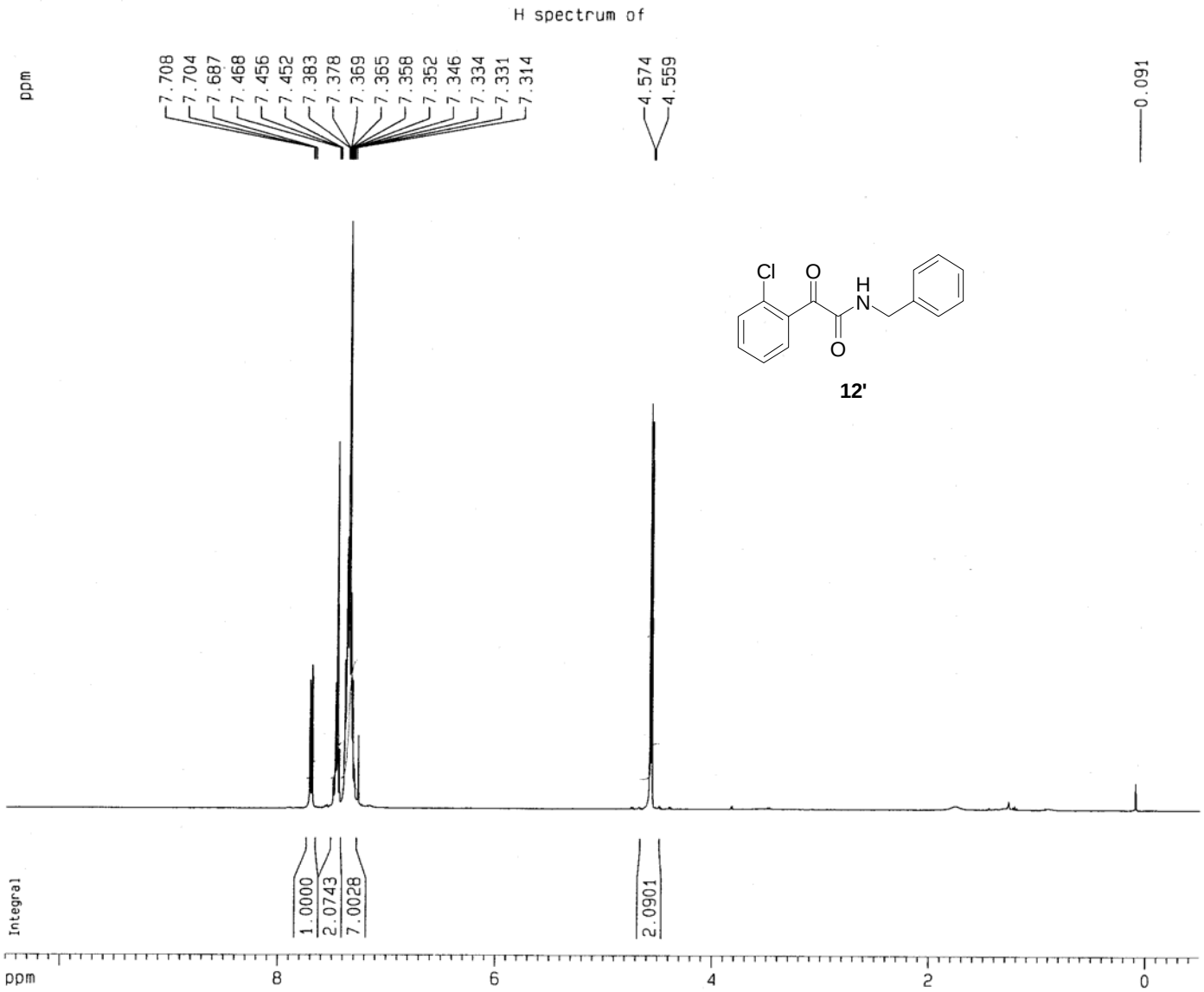

```
Current Data Parameters
NAME          20050608-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_          20050608
Time              15.12
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                16384
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            5995.204 Hz
FIDRES         0.365918 Hz
AQ           1.3664756 sec
RG                  128
DW               83.400 usec
DE                6.50 usec
TE               300.0 K
D1           1.50000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.10 usec
PL1                3.00 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300095 MHz
WDW                  EM
SSB                   0
LB                 0.10 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                10.50 cm
F1P              10.500 ppm
F1              4201.37 Hz
F2P              -0.500 ppm
F2             -200.07 Hz
PPMCM          0.55000 ppm/cm
HZCM         220.07152 Hz/cm
```

C13 spectrum of



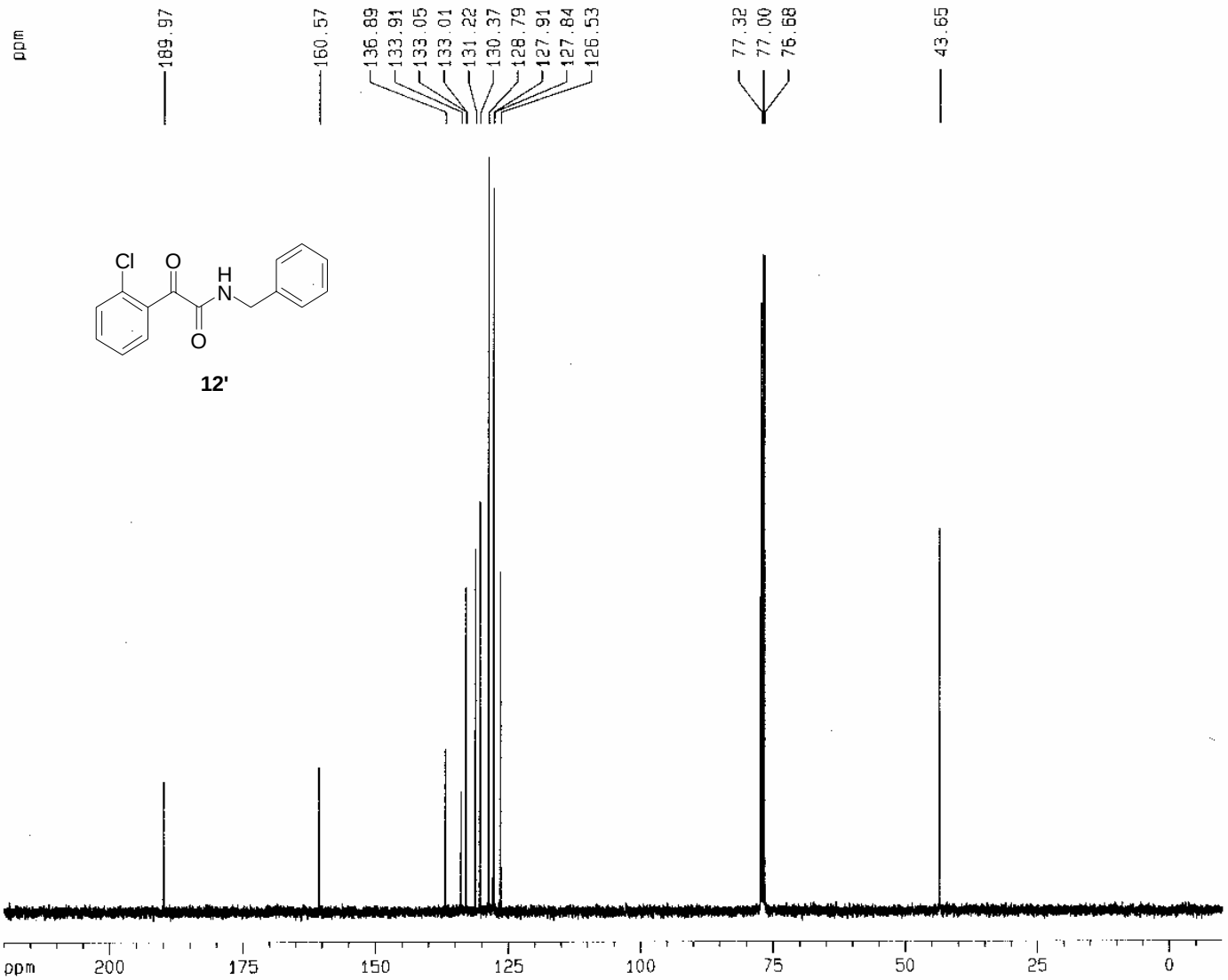
11'

```
Current Data Parameters
NAME          20050608-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20050608
Time              15.15
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  329
DS                    0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ            1.3042164 sec
RG                 8000
DW               19.900 usec
DE                6.50 usec
TE                300.0 K
D1           1.20000005 sec
d11          0.03000000 sec
d12          0.00002000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                10.80 usec
PL1                7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                32768
SF          100.6127744 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                10.00 cm
F1P              240.000 ppm
F1             24147.07 Hz
F2P              -10.000 ppm
F2             -1006.13 Hz
PPMCM            12.50000 ppm/cm
HZCM          1257.65979 Hz/cm
```

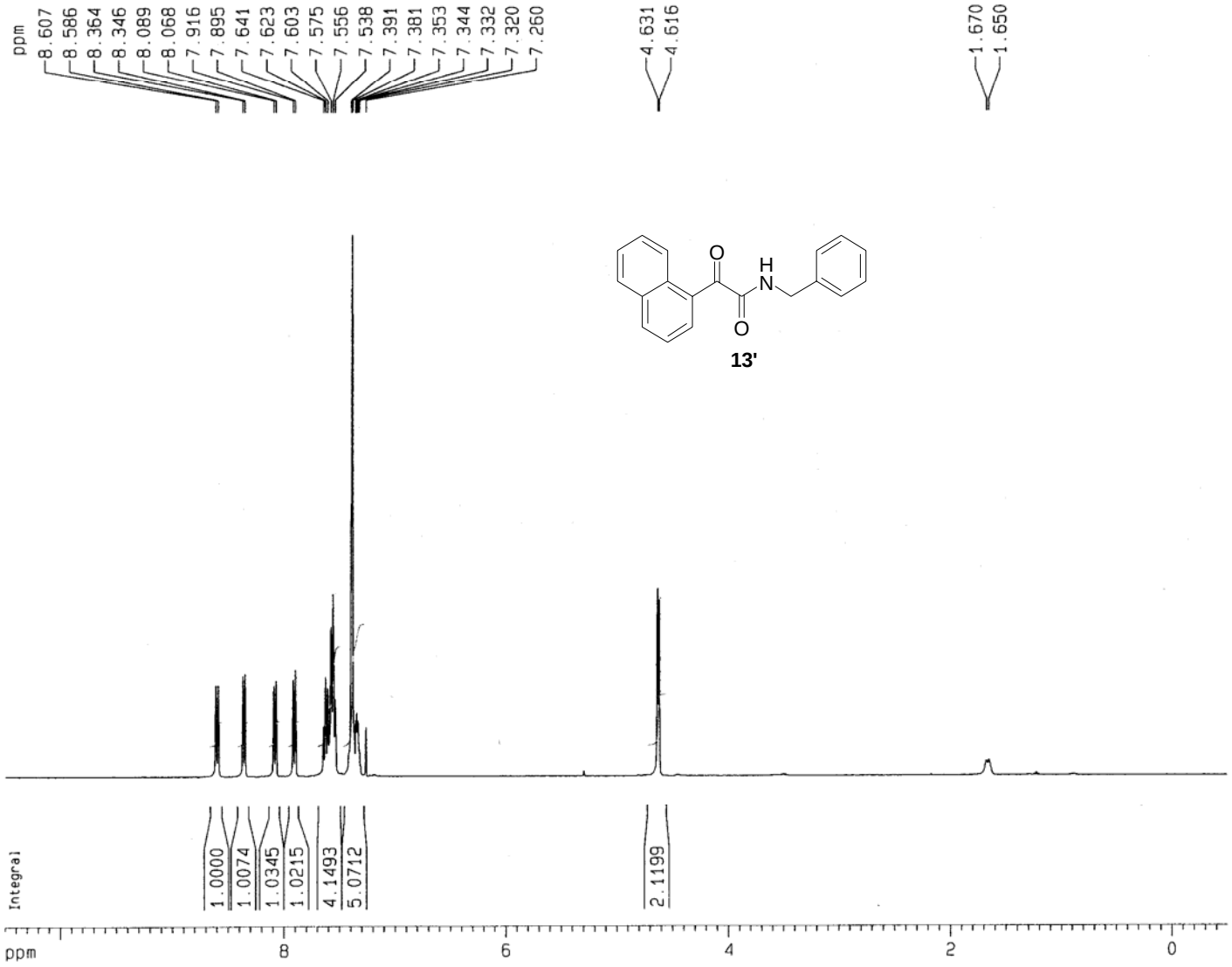



```
Current Data Parameters
NAME        2-Clmedelate
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20050317
Time               12.14
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                     8
DS                     0
SWH            5995.204 Hz
FIDRES         0.365918 Hz
AQ           1.3664756 sec
RG                   114
DW                83.400 usec
DE                 6.50 usec
TE                300.0 K
D1           1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.10 usec
PL1                3.00 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300091 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 10.00 cm
F1P               10.500 ppm
F1               4201.37 Hz
F2P               -0.500 ppm
F2               -200.06 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07150 Hz/cm
```

C13 spectrum of



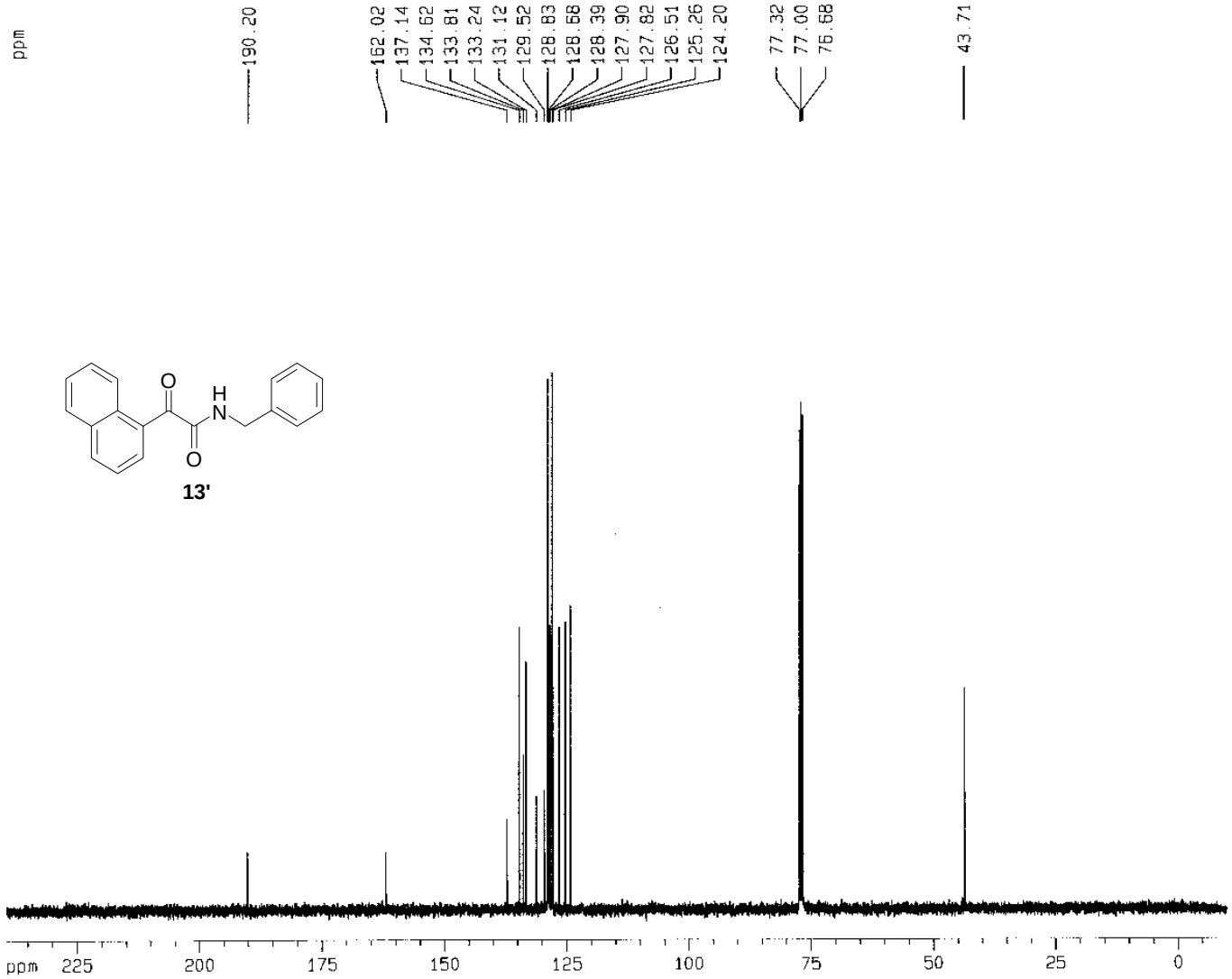

```
Current Data Parameters
NAME        2-Clmedelate
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20050317
Time                12.20
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   244
DS                     0
SWH            25125.629 Hz
FIDRES          0.383387 Hz
AQ             1.3042164 sec
RG                  4096
DW                19.900 usec
DE                 6.50 usec
TE                300.0 K
D1            1.20000005 sec
d11           0.03000000 sec
d12           0.00002000 sec

-------- CHANNEL f1 --------
NUC1                  13C
P1                  10.80 usec
PL1                  7.00 dB
SFO1         100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               90.00 usec
PL2                  3.00 dB
PL12                21.83 dB
PL13                24.80 dB
SFO2         400.1319000 MHz

F2 - Processing parameters
SI                  32768
SF           100.6127782 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                  20.00 cm
CY                  12.50 cm
F1P                220.000 ppm
F1               22134.81 Hz
F2P                -10.000 ppm
F2               -1006.13 Hz
```



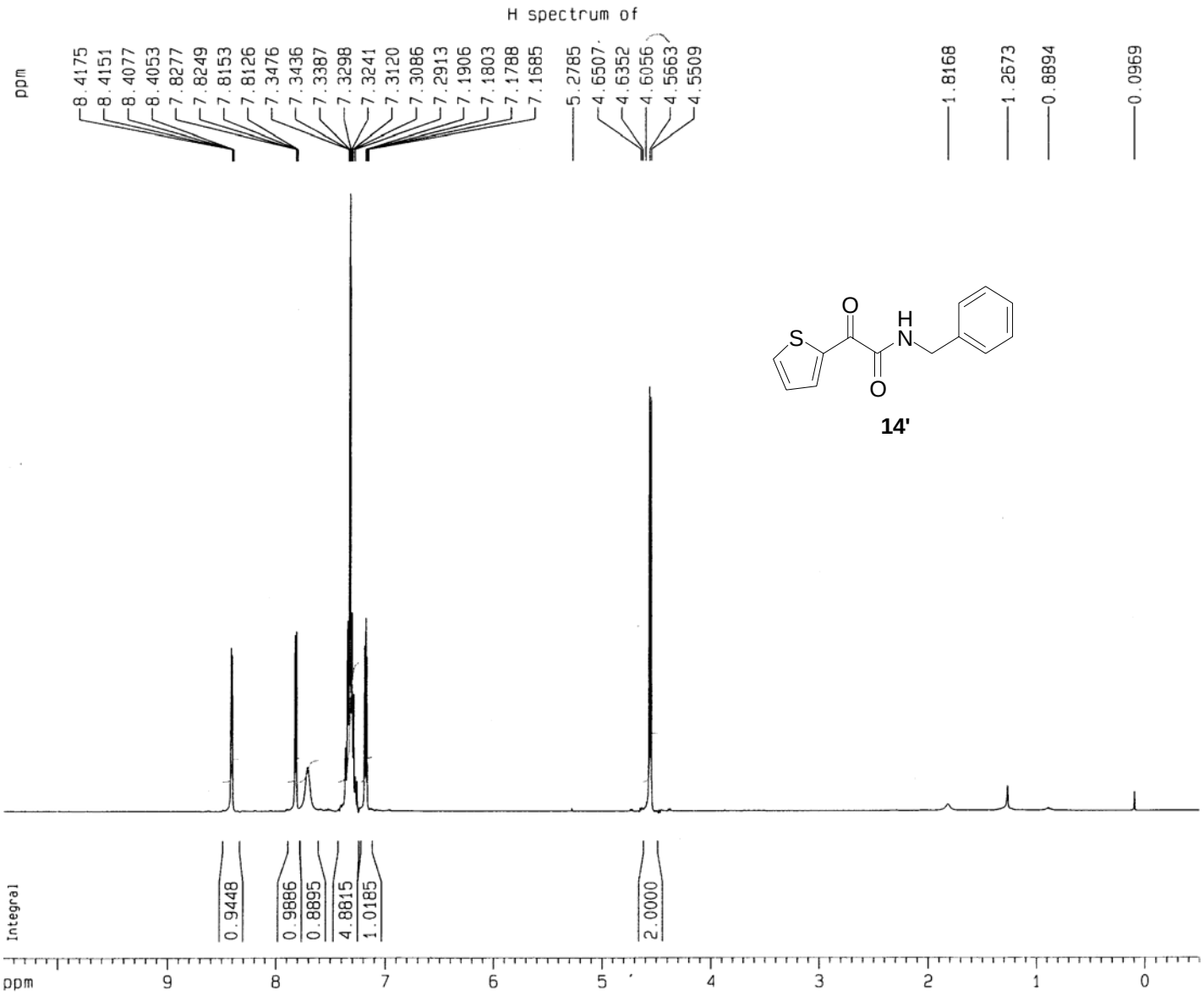
13'

```
Current Data Parameters
NAME      1-naphthylamide
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_           20050310
Time               12.19
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ             1.3664756 sec
RG                  80.6
DW                83.400 usec
DE                  6.50 usec
TE                 300.0 K
D1             1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.10 usec
PL1                 3.00 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300091 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                  9.00 cm
F1P               10.500 ppm
F1               4201.37 Hz
F2P               -0.500 ppm
F2               -200.06 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07150 Hz/cm
```

C13 spectrum of



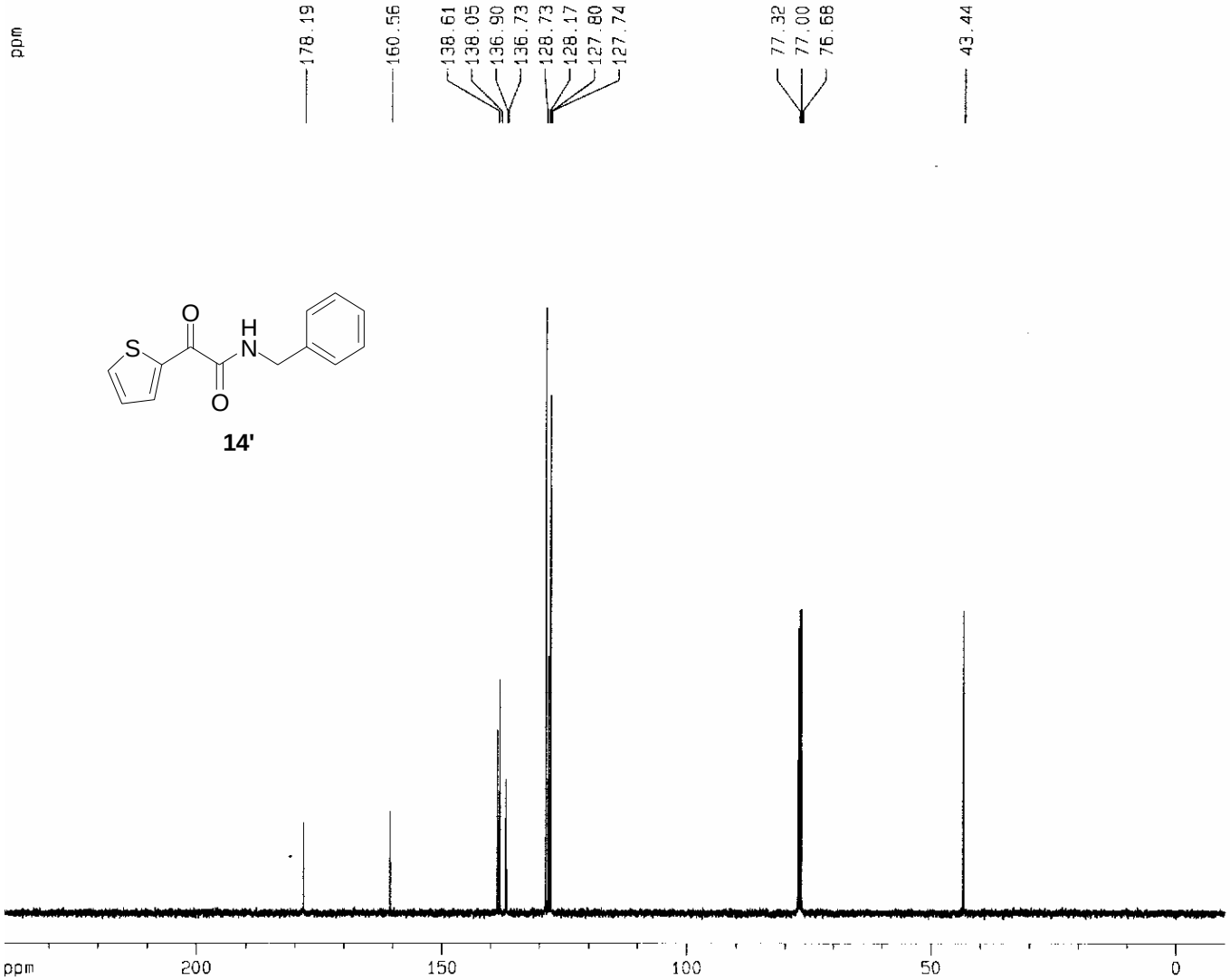

```
Current Data Parameters
NAME      1-naphthylamide
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_           20050310
Time               12.24
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  500
DS                    0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ            1.3042164 sec
RG                 4096
DW               19.900 usec
DE                6.50 usec
TE               300.0 K
D1            1.20000005 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.80 usec
PL1                7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                32768
SF          100.6127775 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                 9.00 cm
F1P              240.000 ppm
F1             24147.07 Hz
F2P              -10.000 ppm
F2             -1006.13 Hz
PPMCM           12.50000 ppm/cm
HZCM          1257.65979 Hz/cm
```



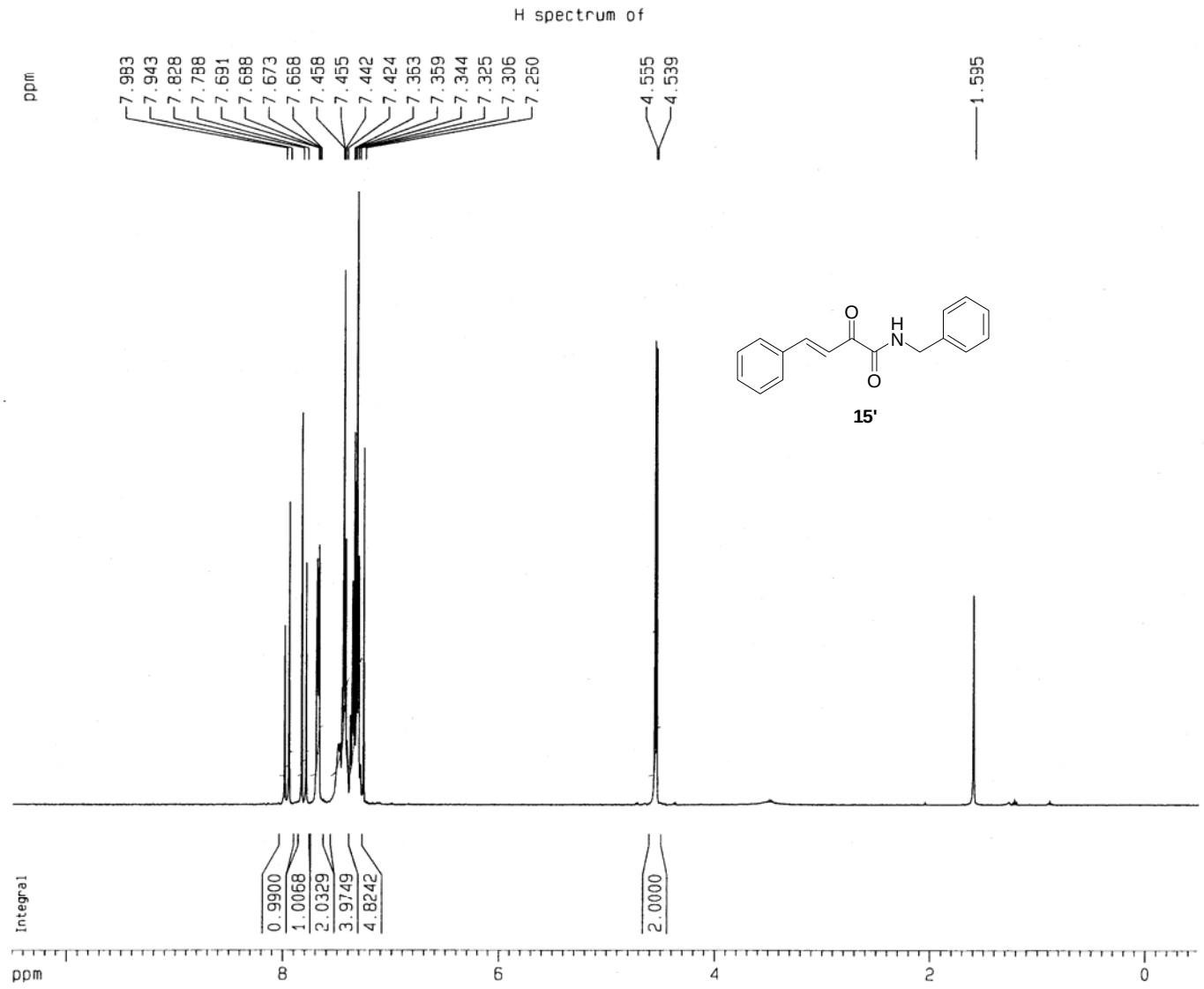
14'

```
Current Data Parameters
NAME          oxidation-3
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20050409
Time                11.01
INSTRUM             spect
PROBHD    5 mm BBO BB-1H
PULPROG              zg30
TD                  16384
SOLVENT             CDCl3
NS                     16
DS                      0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ             1.3664756 sec
RG                   80.6
DW                 83.400 usec
DE                   6.50 usec
TE                  300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.10 usec
PL1                  3.00 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                  16384
SF           400.1300091 MHz
WDW                    EM
SSB                     0
LB                   0.10 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
CY                  10.50 cm
F1P                10.500 ppm
F1                4201.37 Hz
F2P                -0.500 ppm
F2                -200.07 Hz
PPMCM             0.55000 ppm/cm
HZCM            220.07152 Hz/cm
```

C13 spectrum of



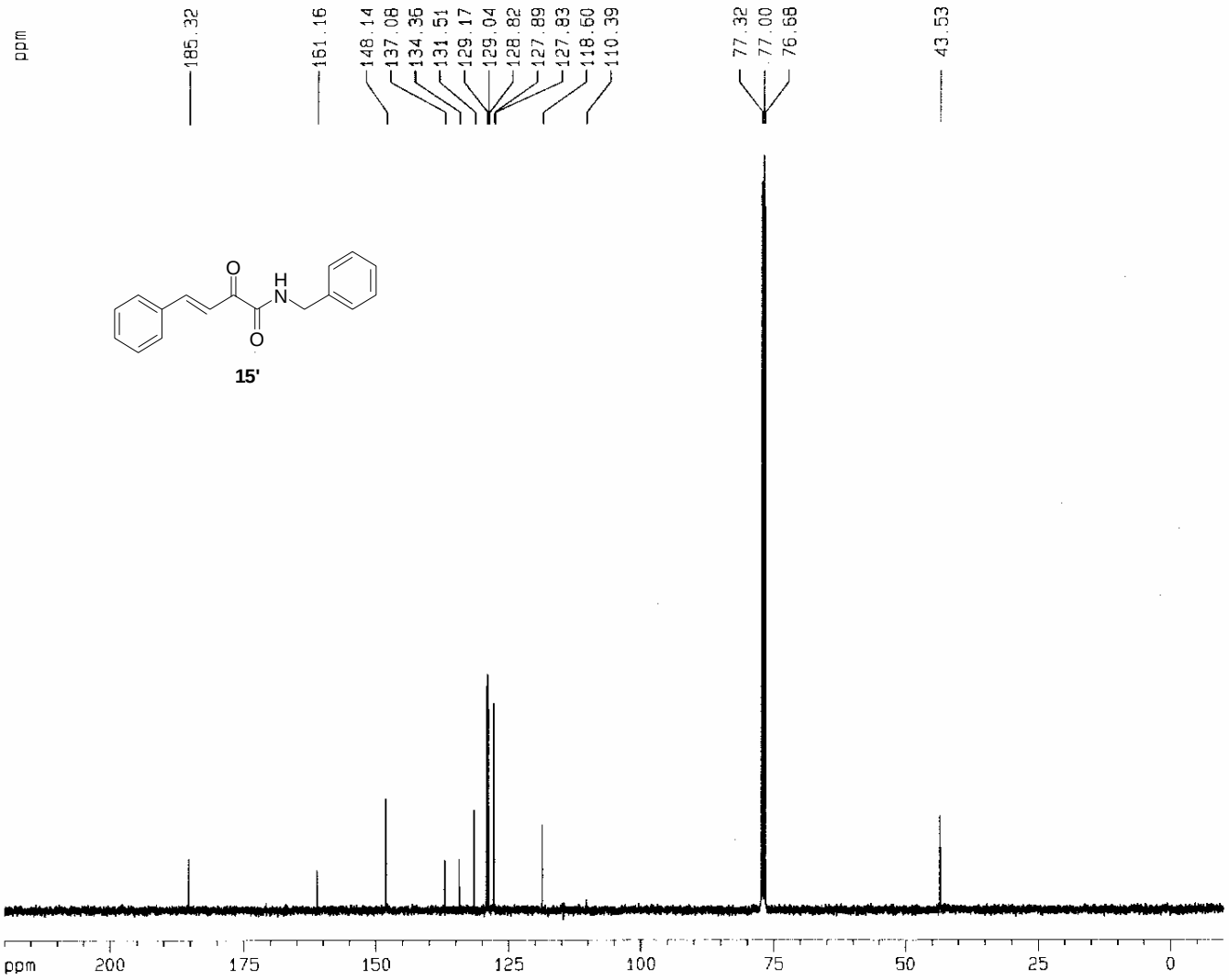

```
Current Data Parameters
NAME          oxidation-3
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20050409
Time                11.05
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     0
SWH            25125.629 Hz
FIDRES          0.383387 Hz
AQ             1.3042164 sec
RG                  8000
DW                19.900 usec
DE                 6.50 usec
TE                300.0 K
D1             1.20000005 sec
d11            0.03000000 sec
d12            0.00002000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                  10.80 usec
PL1                  7.00 dB
SFO1         100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               90.00 usec
PL2                  3.00 dB
PL12                21.83 dB
PL13                24.80 dB
SFO2         400.1319000 MHz

F2 - Processing parameters
SI                  32768
SF           100.6127821 MHz
WDW                    EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 10.00 cm
F1P               240.000 ppm
F1               24147.07 Hz
F2P               -10.000 ppm
F2               -1006.13 Hz
PPMCM            12.50000 ppm/cm
HZCM           1257.65979 Hz/cm
```



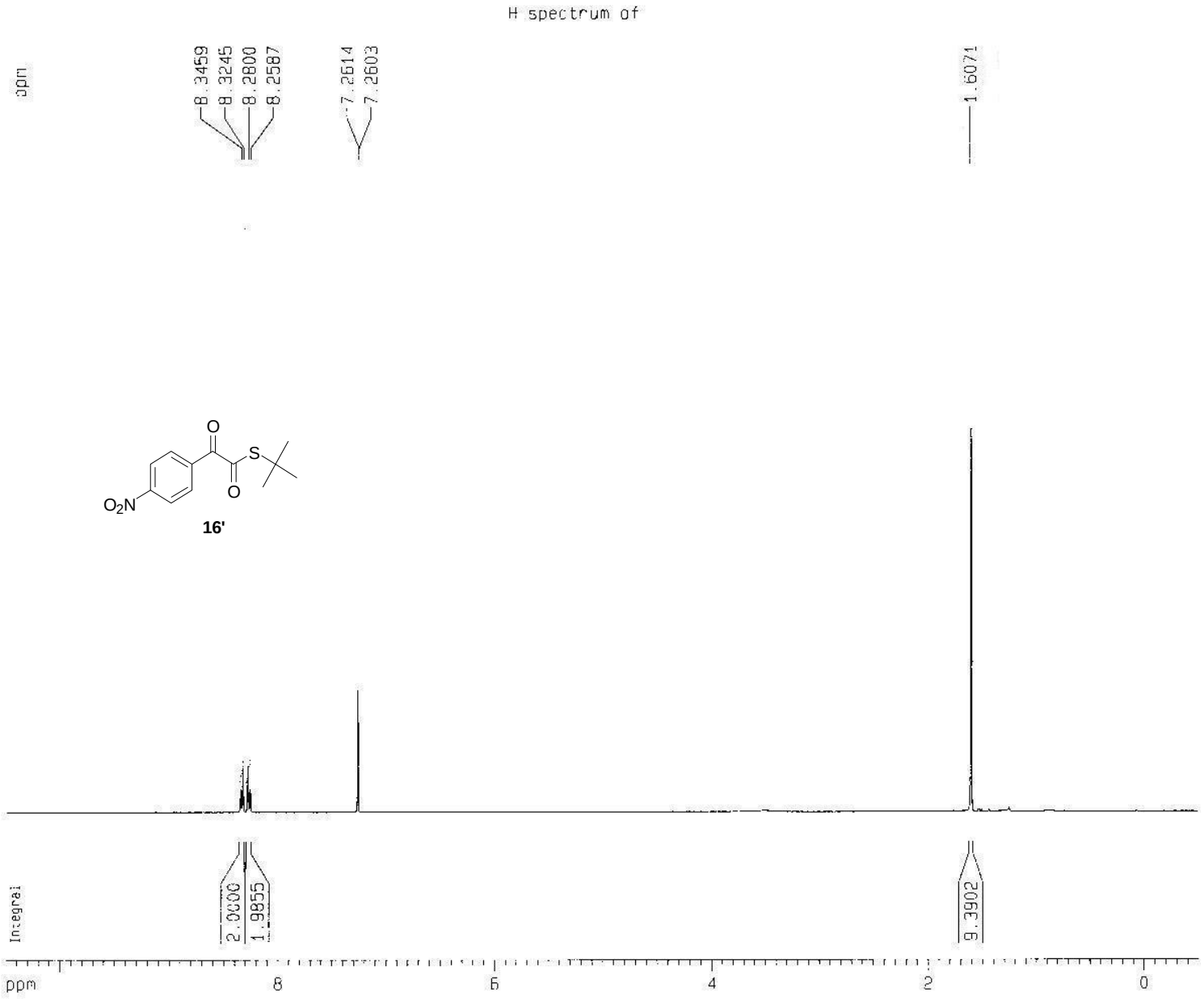
15'

```
Current Data Parameters
NAME      cinamylBnamide
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20050317
Time               12.35
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ             1.3664756 sec
RG                 322.5
DW                83.400 usec
DE                  6.50 usec
TE                 300.0 K
D1             1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.10 usec
PL1                 3.00 dB
SFO1          400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300095 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 10.50 cm
F1P               10.500 ppm
F1               4201.37 Hz
F2P               -0.500 ppm
F2               -200.06 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07150 Hz/cm
```

C13 spectrum of



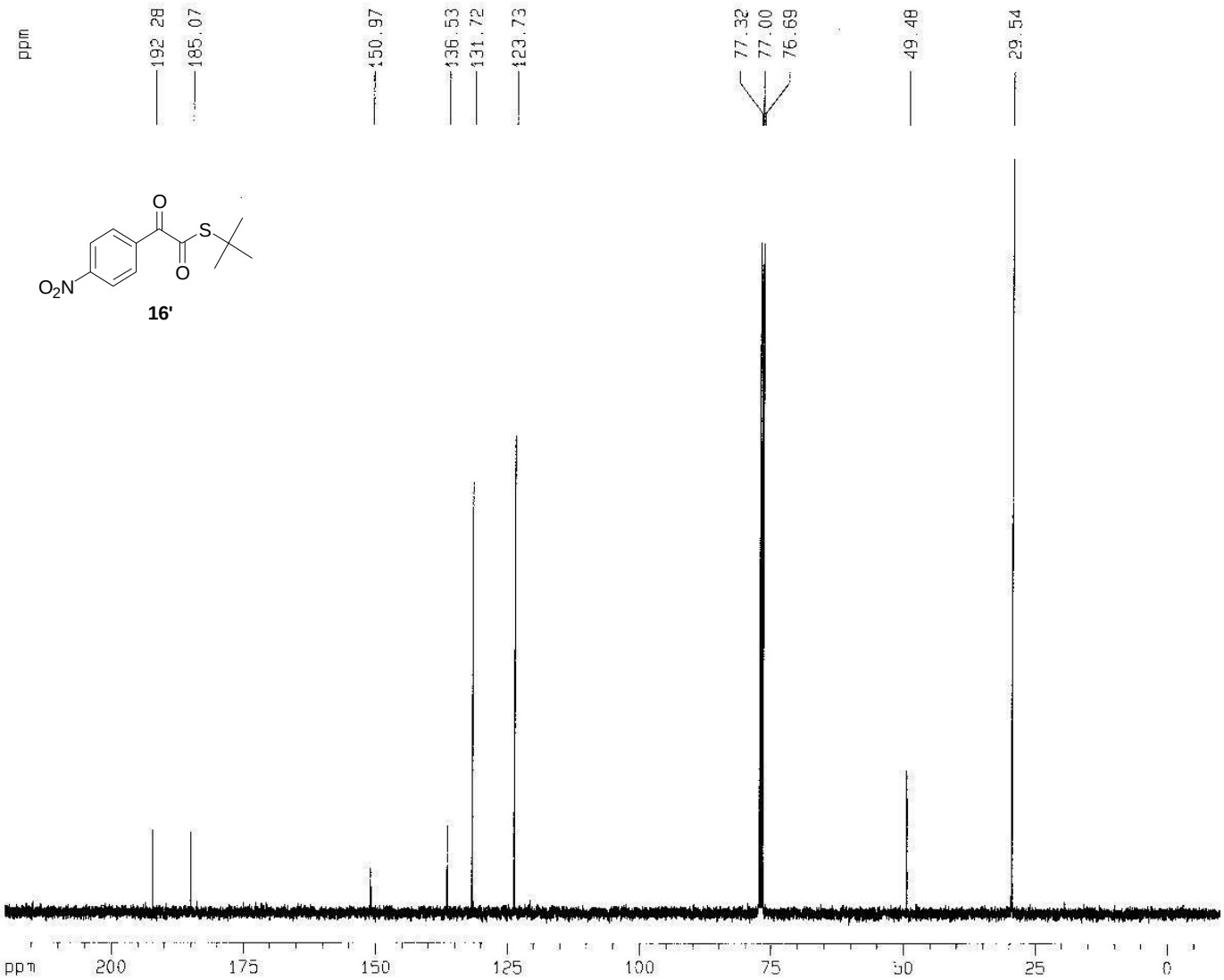

```
Current Data Parameters
NAME      cinamylBnamide
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20050317
Time               12.39
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  623
DS                    0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ            1.3042164 sec
RG                 45.3
DW                19.900 usec
DE                 6.50 usec
TE                300.0 K
D1            1.20000005 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.80 usec
PL1                7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127721 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 12.50 cm
F1P               220.000 ppm
F1              22134.81 Hz
F2P               -10.000 ppm
F2              -1006.13 Hz
PPMCM           11.50000 ppm/cm
HZCM          1157.04688 Hz/cm
```



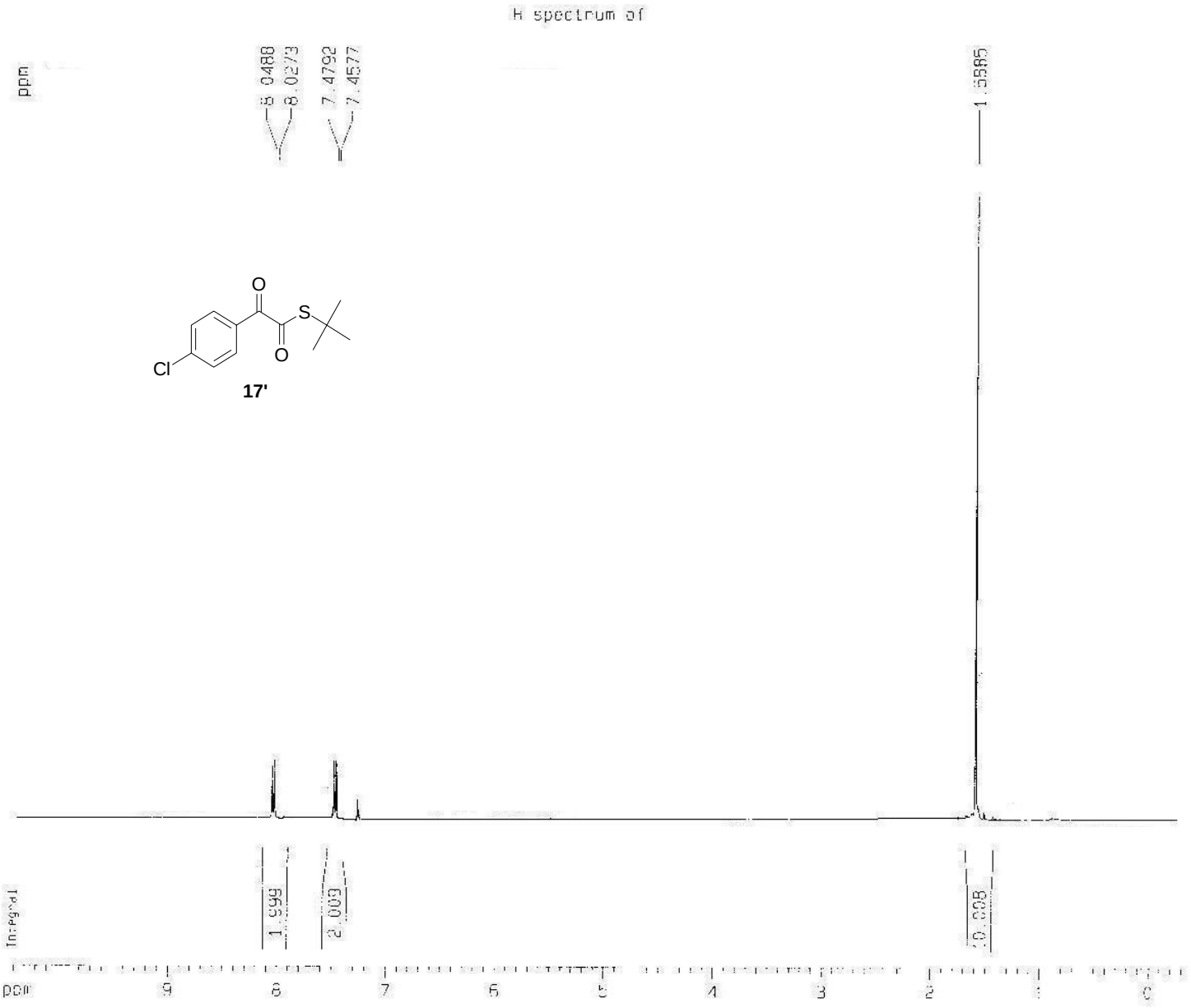
16'

```
NAME      sam 4-Nitro Ket
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20060314
Time               18.55
INSTRUM            spect
PROBHD  5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ             1.3664756 sec
RG                 645.1
DW                83.400 usec
DE                 6.50 usec
TE                300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.10 usec
PL1                 3.00 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300091 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                  6.50 cm
F1P               10.500 ppm
F1               4201.37 Hz
F2P               -0.500 ppm
F2               -200.05 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07150 Hz/cm
```

C13 spectrum of



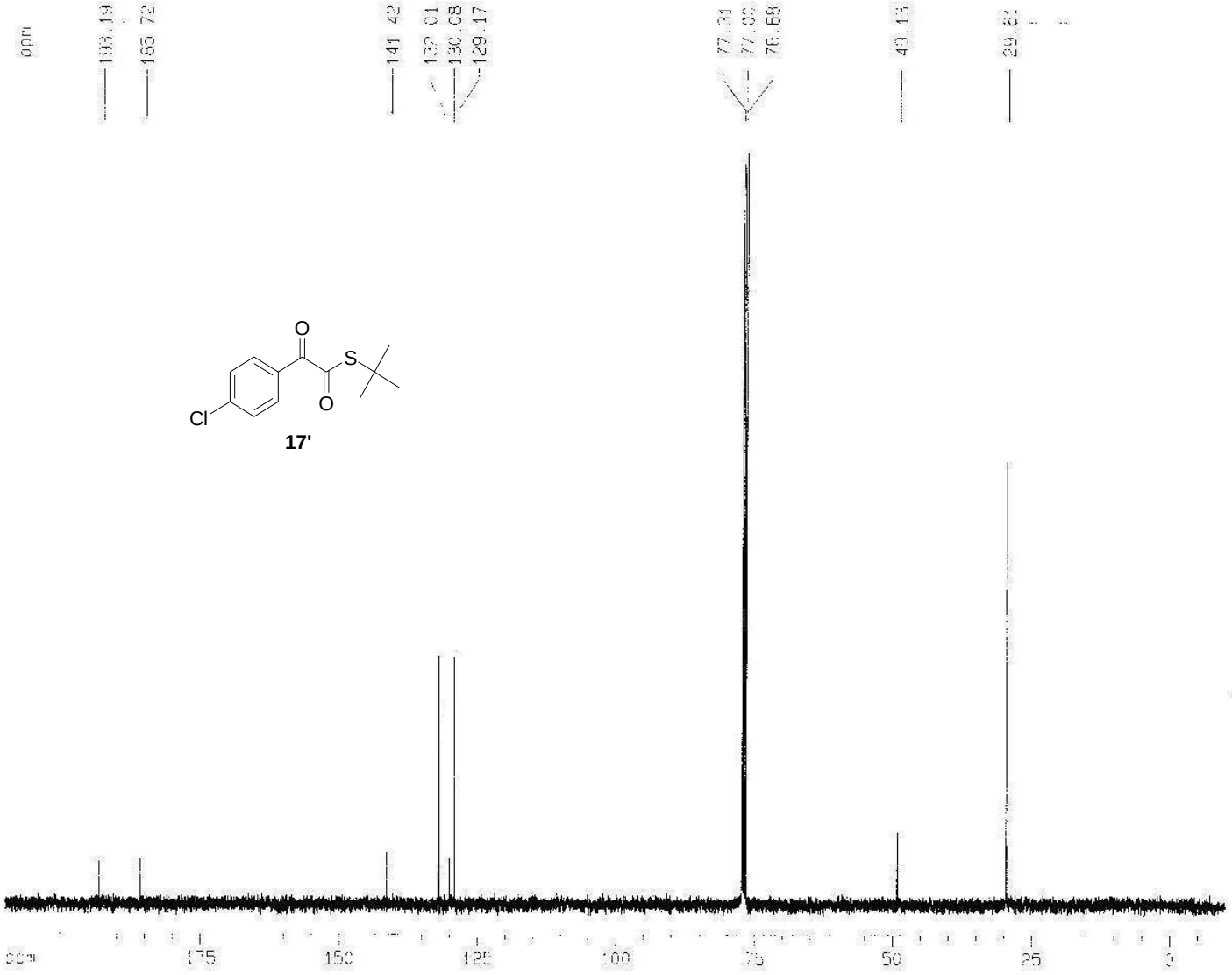

```
Current Data Parameters
NAME      sam-4-nitrketC
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20060314
Time               16 30
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  214
DS                    0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ            1.3042164 sec
RG                 8192
DW               19.900 usec
DE                6.50 usec
TE               300.0 K
D1            1.20000005 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1                7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                32768
SF          100.6127721 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                12.50 cm
F1P              220.000 ppm
F1             22134.81 Hz
F2P              -10.000 ppm
F2             -1005.13 Hz
PPMCM           11.50000 ppm/cm
HZCM          1157.04688 Hz/cm
```



17'

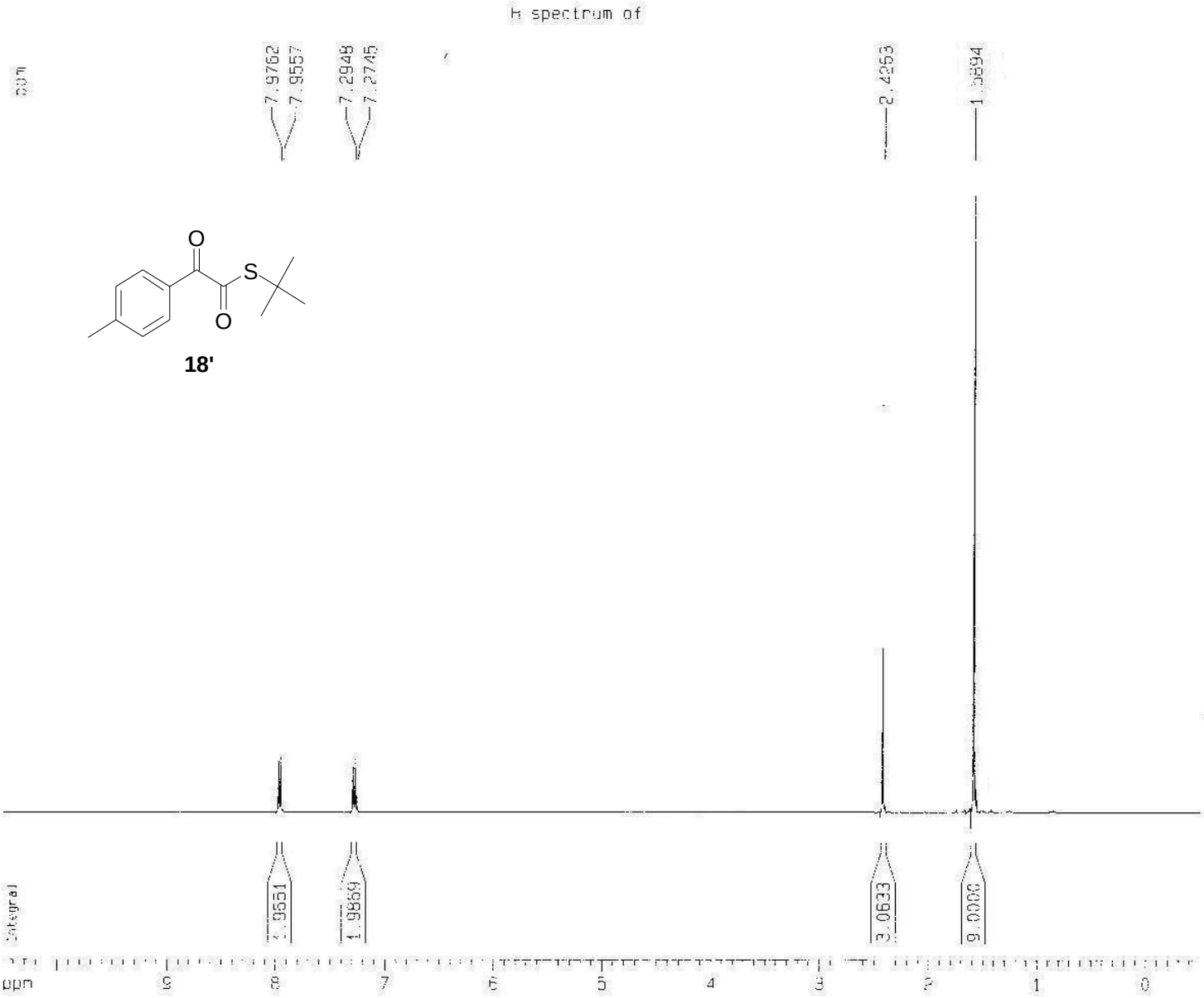
```
NAME        4-Cl thio ket
EXPNO                   1
PROCNO                  1

-2 - Acquisition Parameters
Date_           20060210
Time               11.05
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ              1.3664756 sec
RG                    256
DW                 83.400 usec
DE                  6.50 usec
TE                 300.0 K
D1              1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.10 usec
PL1                 3.00 dB
SFO1          400.1326008 MHz

-2 - Processing parameters
SI                 16384
SF            400.1300095 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 10.50 cm
F1P               10.500 ppm
F1                4201.37 Hz
F2P               -0.500 ppm
F2                -200.07 Hz
PPMCM             0.55000 ppm/cm
HZCM            220.07152 Hz/cm
```

C13 spectrum of

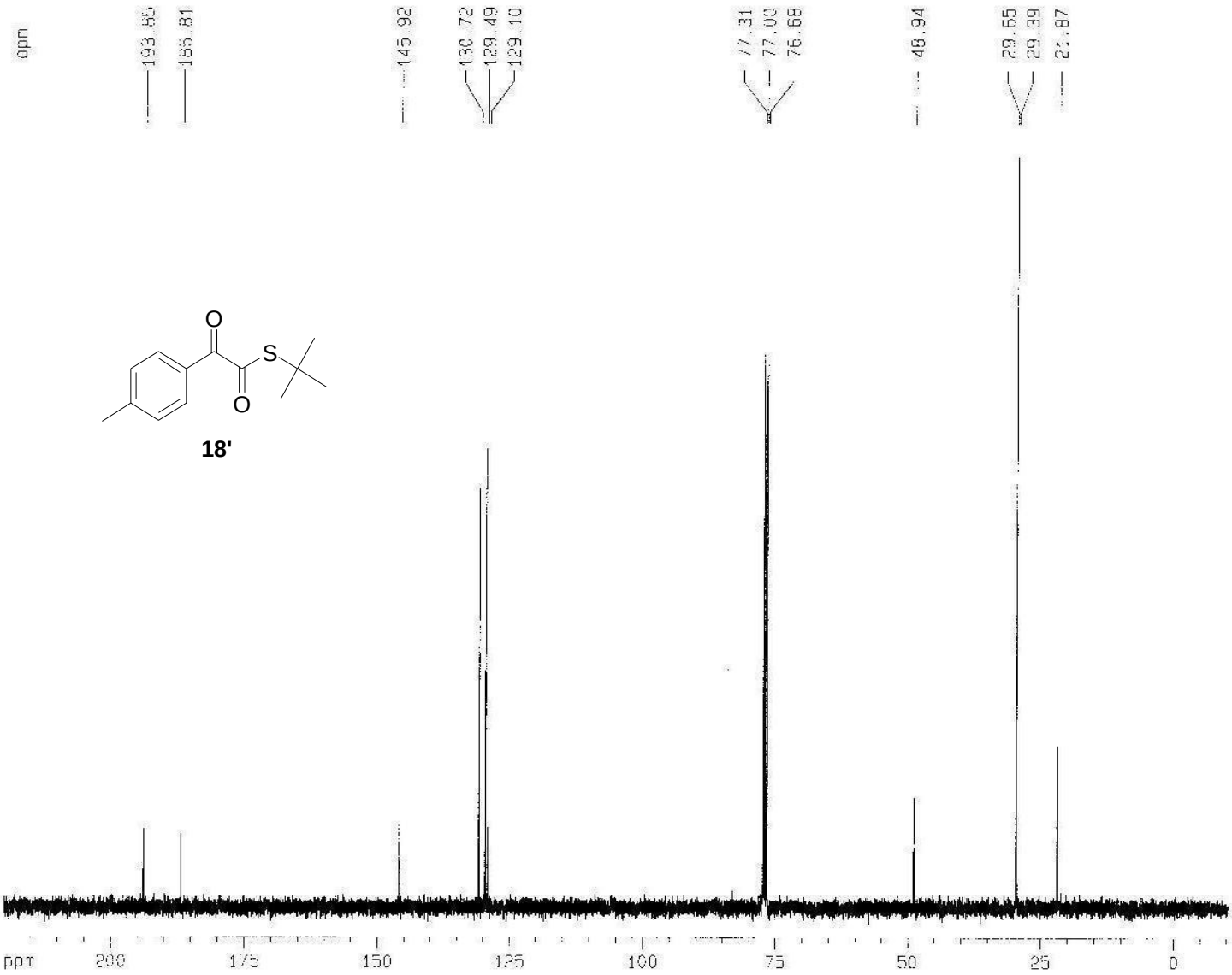



```
Current Data Parameters
NAME      sam_4_01_f310-ket
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_          20060210
Time              12 19
INSTRUM           spect
PROBHD   5 mm BBO 30 1H
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                  200
DS                    2
SWH           25125.629 Hz
FIDRES        0.383387 Hz
AQ            1.3042164 sec
RG               322.5
DW               19.900 usec
DE                6.50 usec
TE               300.0 K
D1            1.20000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1               13C
P1               10.80 usec
PL1               7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2               1H
PCPD2            90.00 usec
PL2               3.00 dB
PL12             21.93 dB
PL13             24.50 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI               32768
SF          100.6127713 MHz
WDW               EM
SSB                0
LB                1.00 Hz
GB                 0
PC                1.40

1D NMR plot parameters
CX               20.00 cm
CY               19.50 cm
F1P             210.000 ppm
F1             21126.08 Hz
F2P             -10.000 ppm
F2             -1006.13 Hz
PPMCM           11.00000 ppm/cm
HZCM          1106.74040 Hz/cm
```

18'

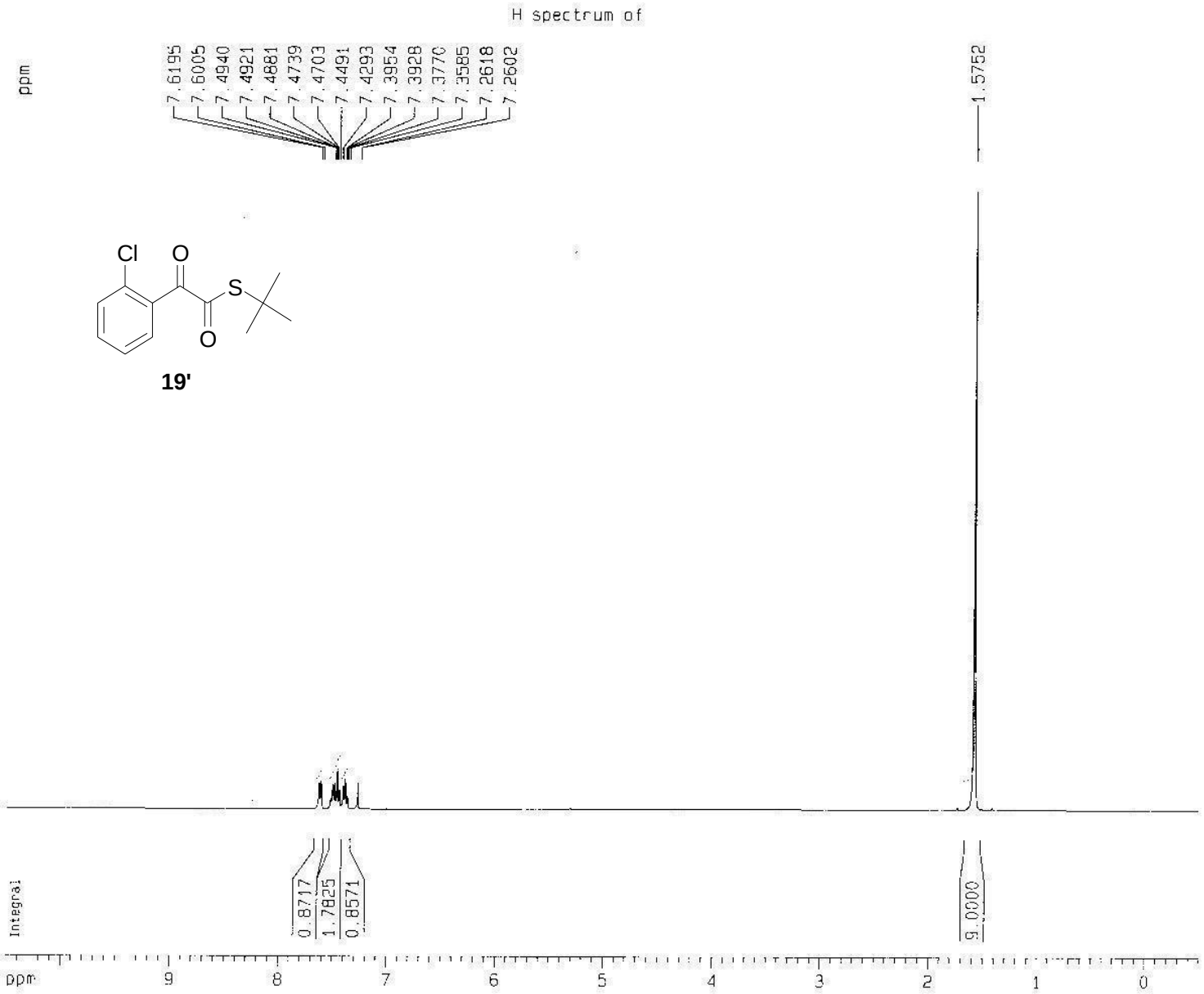



```
NAME                 1
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date           20080211
Time              14.18
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                16384
SOLVENT           CDCl3
NS                    1
DS                    0
SWH            5995.204 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                 22.6
DW               83.400 usec
DE                6.50 usec
TE                300.0 K
D1           1.50000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.10 usec
PL1               3.00 dB
SFO1        400.1326006 MHz

F2 - Processing parameters
SI                16384
SF          400.1300095 MHz
WDW                  EM
SSB                   0
LB                 0.10 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                10.50 cm
F1P              10.500 ppm
F1              4201.37 Hz
F2P              -0.500 ppm
F2              -200.07 Hz
PPMCM          0.95000 ppm/cm
HZCM         220.07152 Hz/cm
```



18'

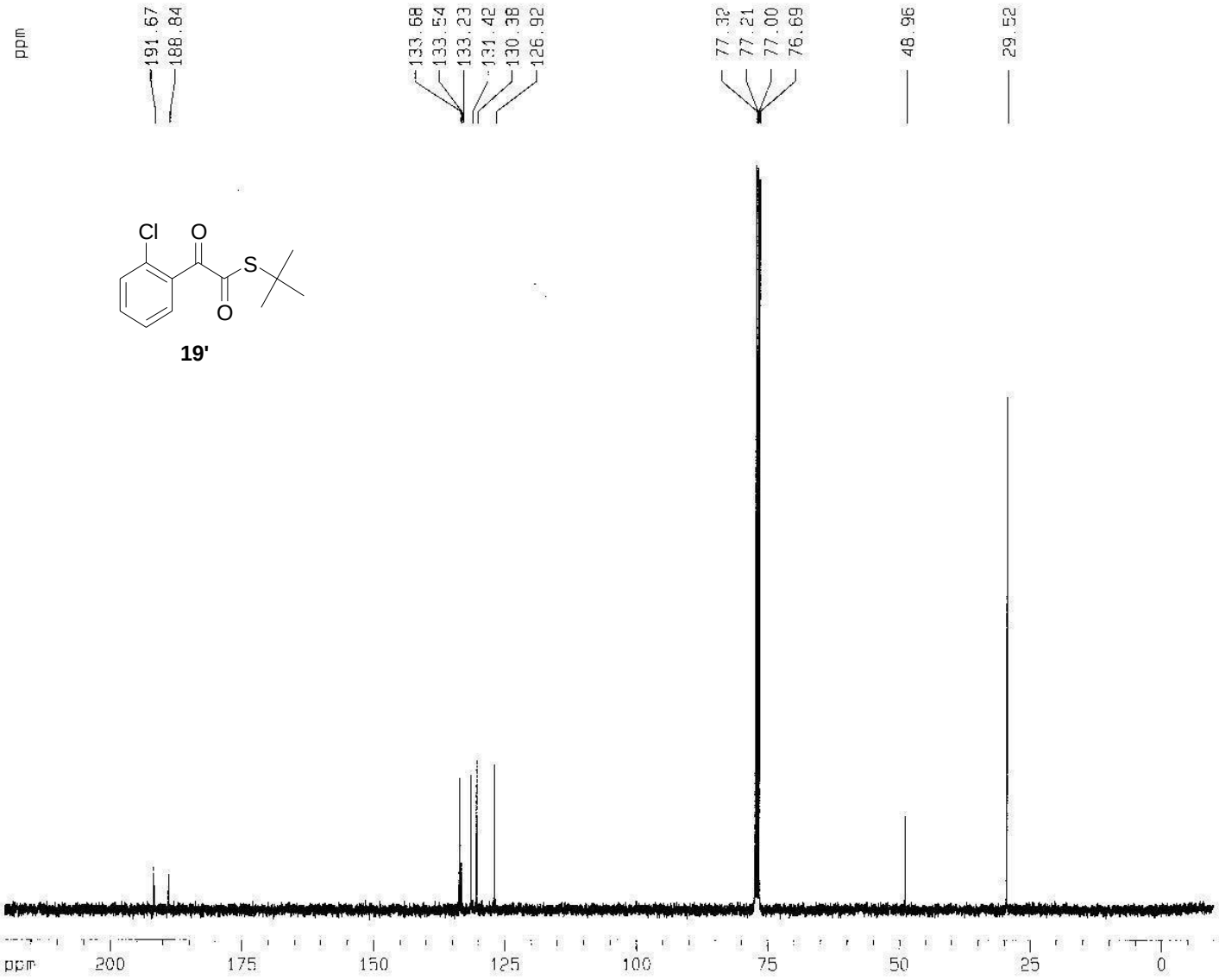
```
Current Data Parameters
NAME      4-Me thioketone
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20060211
Time               15.04
INSTRUM            spect
PROBHD   5 mm BBO BB 1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   60
DS                    0
SWH            25125.629 Hz
FIDRES          0.383367 Hz
AQ             1.3042164 sec
RG                  8192
DW                19.900 usec
DE                 6.50 usec
TE                300.0 K
D1             1.20000000 sec
d11            0.03000000 sec
d12            0.00002000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PL1                 7.00 dB
SFO1          100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 3.00 dB
PL12               23.83 dB
PL13               24.80 dB
SFO2          400.1319000 MHz

F2 - Processing parameters
SI                 32768
SF            100.6127736 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 12.50 cm
F1P               220.000 ppm
F1                22134.81 Hz
F2P                -10.307 ppm
F2                -1036.97 Hz
PPMCM             11.51533 ppm/cm
HZCM           1158.59867 Hz/cm
```



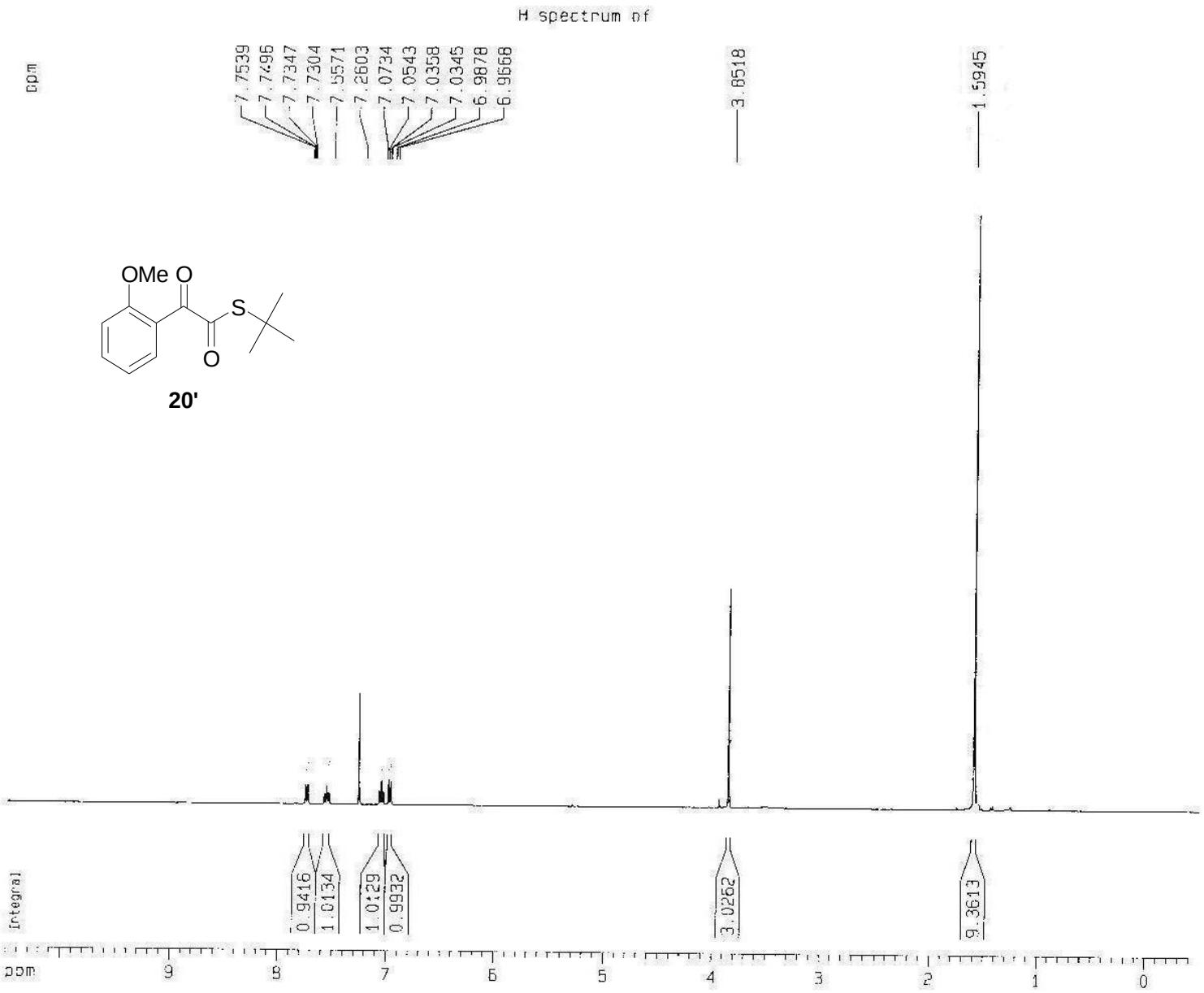
19'

```
Current Data Parameters
NAME      sam-2-Cl-HT-Ket
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20060528
Time               17.35
INSTRUM            spect
PROBHD   5 mm 880 BB-1H
PULPROG            zg30
TD                16384
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            5995.204 Hz
FIDRES         0.365918 Hz
AQ           1.3664756 sec
RG               228.1
DW              83.400 usec
DE                6.50 usec
TE               300.0 K
D1           1.50000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.10 usec
PL1                3.00 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300080 MHz
WDW                  EM
SSB                   0
LB                 0.10 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                10.50 cm
F1P              10.500 ppm
F1              4201.37 Hz
F2P              -0.500 ppm
F2              -200.07 Hz
PPMCM           0.55000 ppm/cm
HZCM          220.07152 Hz/cm
```

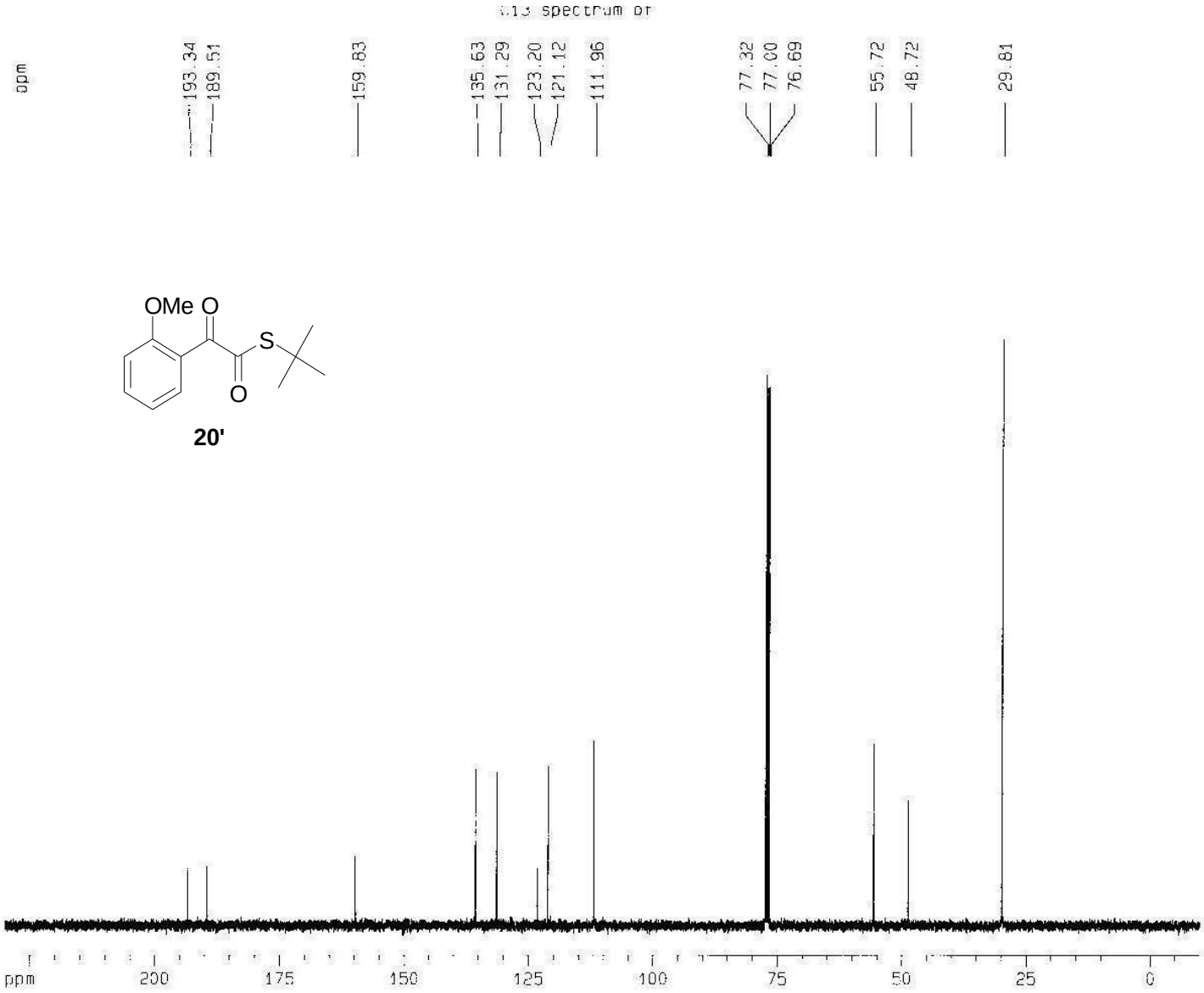
C13 spectrum of




```
Current Data Parameters
NAME      sam-2-C1-HT-Ket
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20060528
Time                17.35
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   500
DS                     0
SWH            25125.629 Hz
FIDRES          0.383387 Hz
AQ             1.3042164 sec
RG                  4096
DW                19.900 usec
DE                 6.50 usec
TE                300.0 K
D1             1.20000005 sec
d11            0.03000000 sec
d12            0.00002000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.80 usec
PL1                 7.00 dB
SFO1          100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 3.00 dB
PL12               21.83 dB
PL13               24.90 dB
SFO2          400.1319000 MHz

F2 - Processing parameters
SI                 32768
SF            100.6127706 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 12.50 cm
F1P               220.000 ppm
F1              22134.81 Hz
F2P               -10.000 ppm
F2              -1006.13 Hz
PPMCM             11.50000 ppm/cm
HZCM            1157.04688 Hz/cm
```

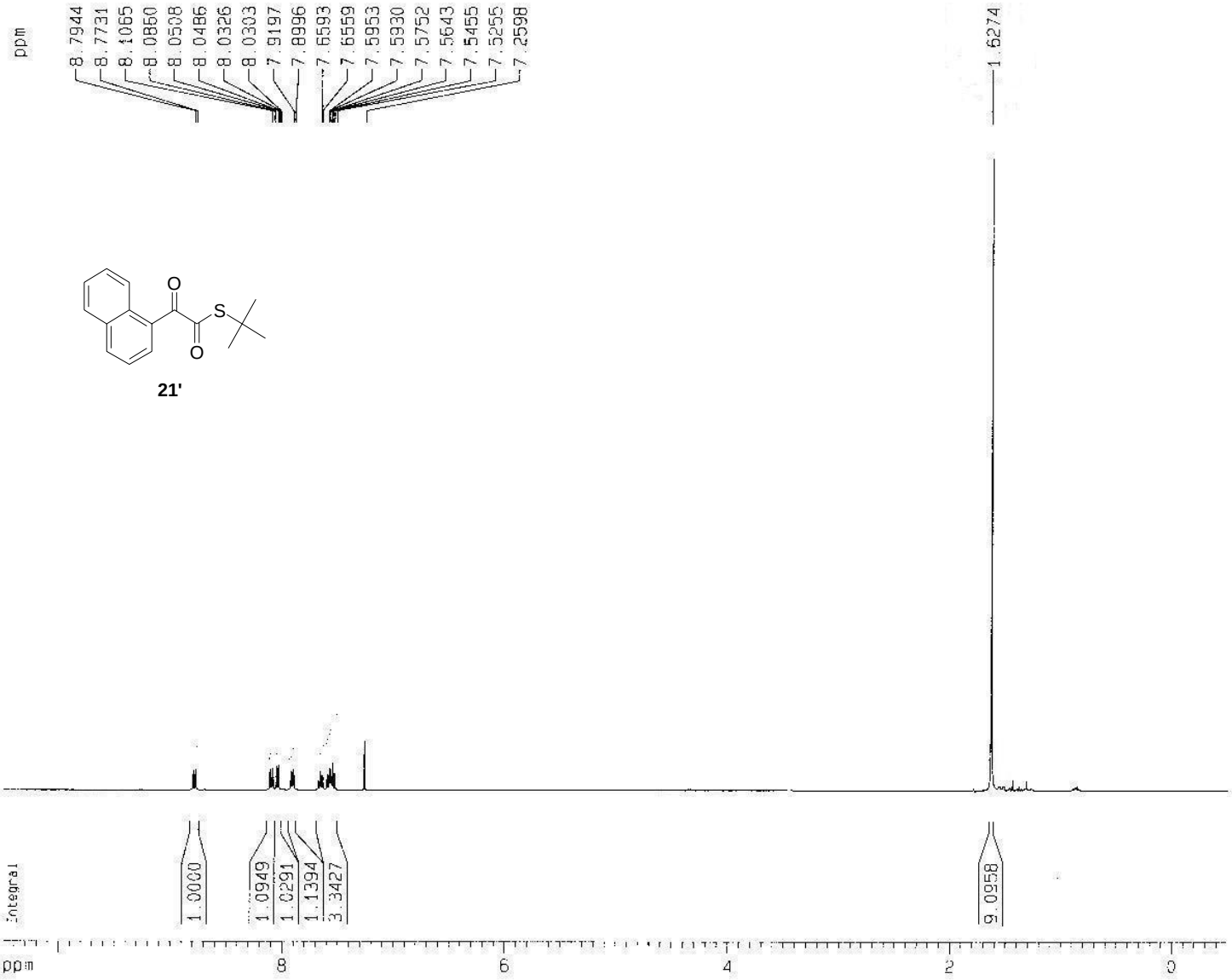



```
Current Data Parameters
NAME        sam-2-Ome-Ket
EXPNO               1
PROCNO              1

F2 - Acquisition Parameters
Date_          20060311
Time              12.28
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                15384
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            5995.204 Hz
FIDRES         0.36591B Hz
AQ            1.3664756 sec
RG               574.7
DW               83.400 usec
DE                5.50 usec
TE               300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1               10.10 usec
PL1               3.00 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300095 MHz
WDW                  EM
SSB                   0
LB               0.10 Hz
GB                    0
PC                1.00

1D NMR plot parameters
CX               20.00 cm
CY               10.50 cm
F1P              10.500 ppm
F1             4201.37 Hz
F2P              -0.500 ppm
F2             -200.07 Hz
PPMCM          0.55000 ppm/cm
HZCM         220.07152 Hz/cm
```




```
Current Data Parameters
NAME      sam TH-2-OMe ket
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20060311
Time               17.13
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  181
DS                    0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ            1.3042164 sec
RG               3649.1
DW               19.900 usec
DE                 6.50 usec
TE                300.0 K
D1            1.20000005 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.80 usec
PL1                7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                32768
SF          100.6127729 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                10.00 cm
F1P              230.000 ppm
F1             23140.94 Hz
F2P              -10.000 ppm
F2             -1006.13 Hz
PPMCM           12.00000 ppm/cm
HZCM          1207.35315 Hz/cm
```

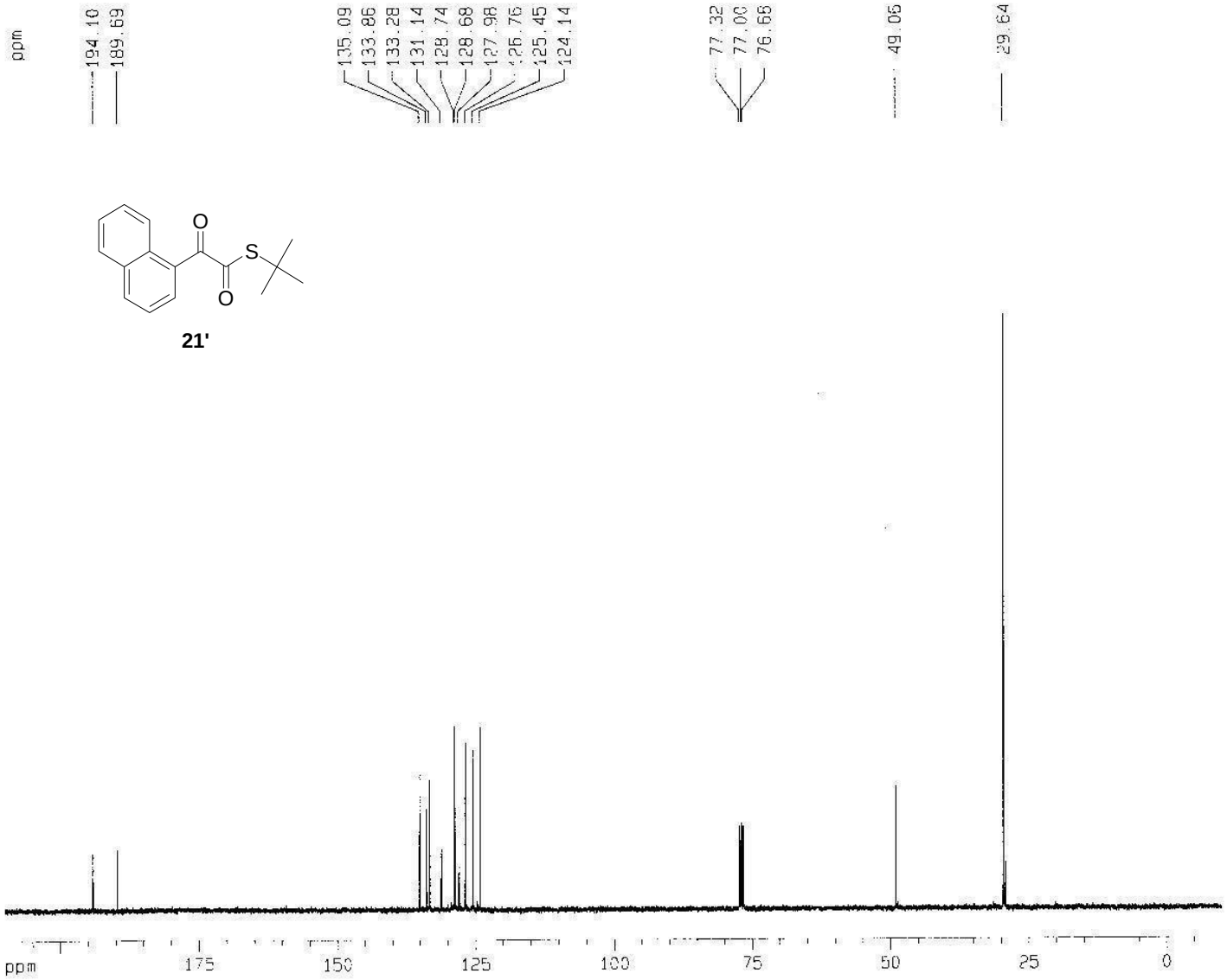
H spectrum of



21'

```
Current Data Parameters
NAME          sam-Nap-ket
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20060426
Time               18 46
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             5995.204 Hz
FIDRES          0.365918 Hz
AQ            1.3664756 sec
RG                 287.4
DW                83.400 usec
DE                  6.50 usec
TE                 300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.10 usec
PL1                 3.00 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300095 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 10.50 cm
F1P               10.500 ppm
F1               4201.37 Hz
F2P               -0.500 ppm
F2               -200.06 Hz
PPMCM            0.55000 ppm/cm
HZCM           220.07150 Hz/cm
```

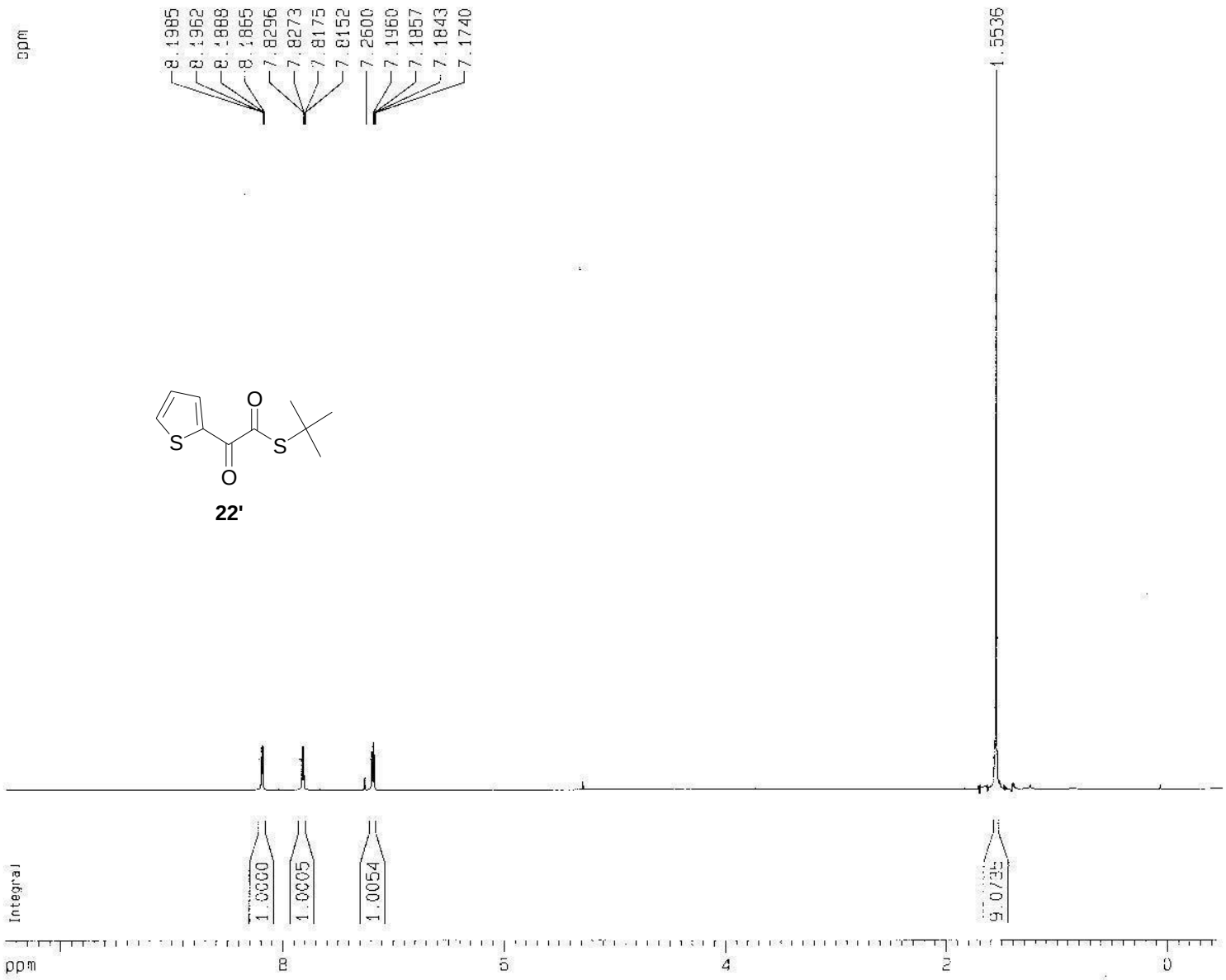
C13 spectrum of



21'

```
Current Data Parameters
NAME              TH-Nap
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20060321
Time               14.31
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  109
DS                    0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ            1.3042164 sec
RG                 6192
DW               19.900 usec
DE                6.50 usec
TE                300.0 K
D1            1.20000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.80 usec
PL1                7.00 dB
SFO1        100.6242895 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2            90.00 usec
PL2               3.00 dB
PL12             21.83 dB
PL13             24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127758 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 10.00 cm
F1P               210.000 ppm
F1                21128.68 Hz
F2P               -10.000 ppm
F2                -1006.13 Hz
PPMCM             11.00000 ppm/cm
HZCM            1105.74048 Hz/cm
```

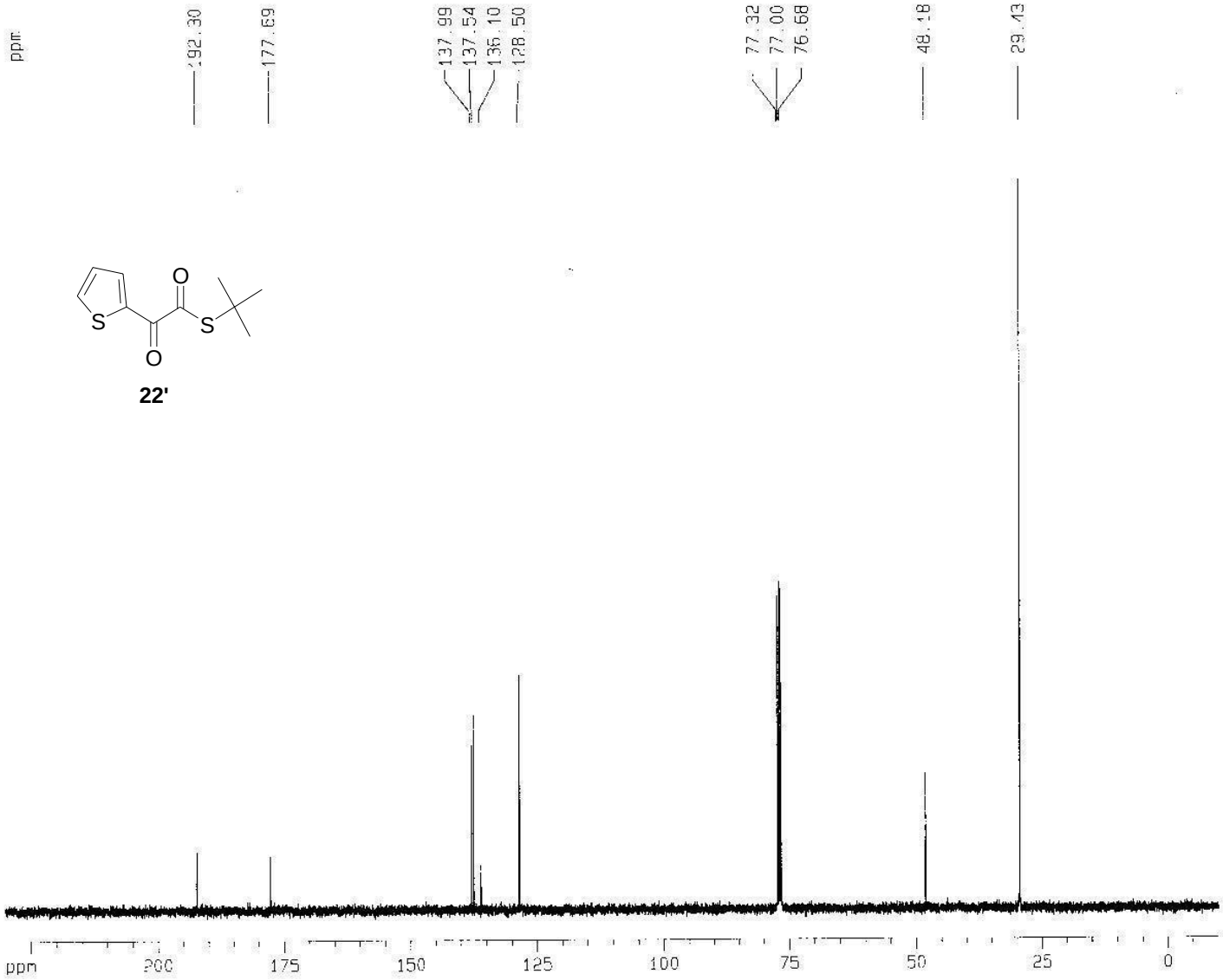
H spectrum of



22'

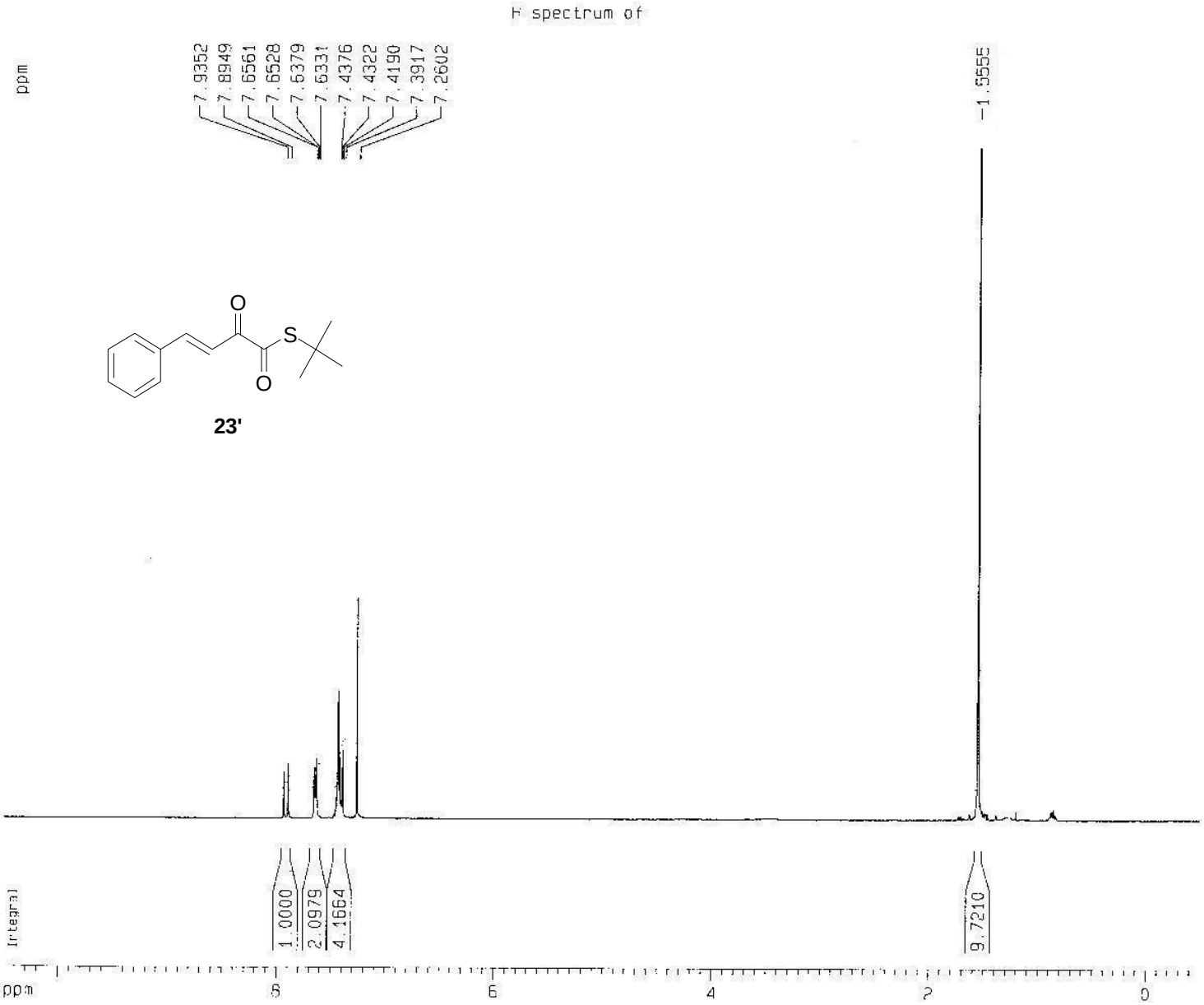
```
NAME        sam-thio-ket
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20060422
Time               17.43
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT            CDCl3
NS                     1
DS                     0
SWH            5995.204 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                 101.6
DW                83.400 usec
DE                 6.50 usec
TE                300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                10.10 usec
PL1                3.00 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300095 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 15.00 cm
F1P               10.500 ppm
F1              4201.37 Hz
F2P               -0.500 ppm
F2              -200.06 Hz
PPMCM           0.55000 ppm/cm
HZCM          220.07150 Hz/cm
```

C13 spectrum of



22'

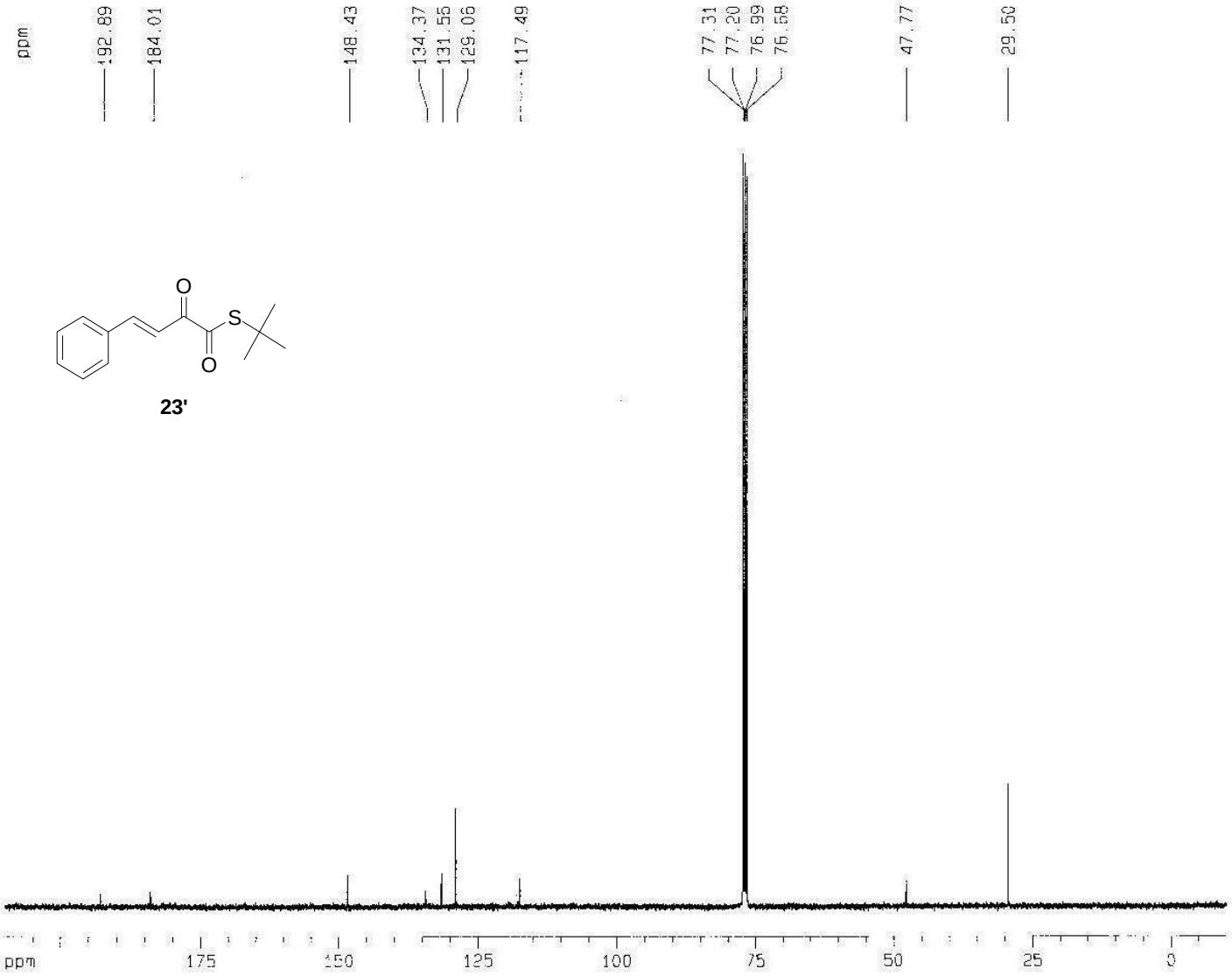
```
Current Data Parameters
NAME        sam thio-xet
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20060422
Time              17.49
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  118
DS                    0
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ             1.3042164 sec
RG                 8192
DW               19.900 usec
DE                6.50 usec
TE                300.0 K
D1            1.20000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.80 usec
PL1                7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.83 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127744 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 12.50 cm
F1P             230.000 ppm
F1             23140.94 Hz
F2P             -10.000 ppm
F2             -1006.13 Hz
PPMCM          12.00000 ppm/cm
HZCM         1207.35327 Hz/cm
```



23'

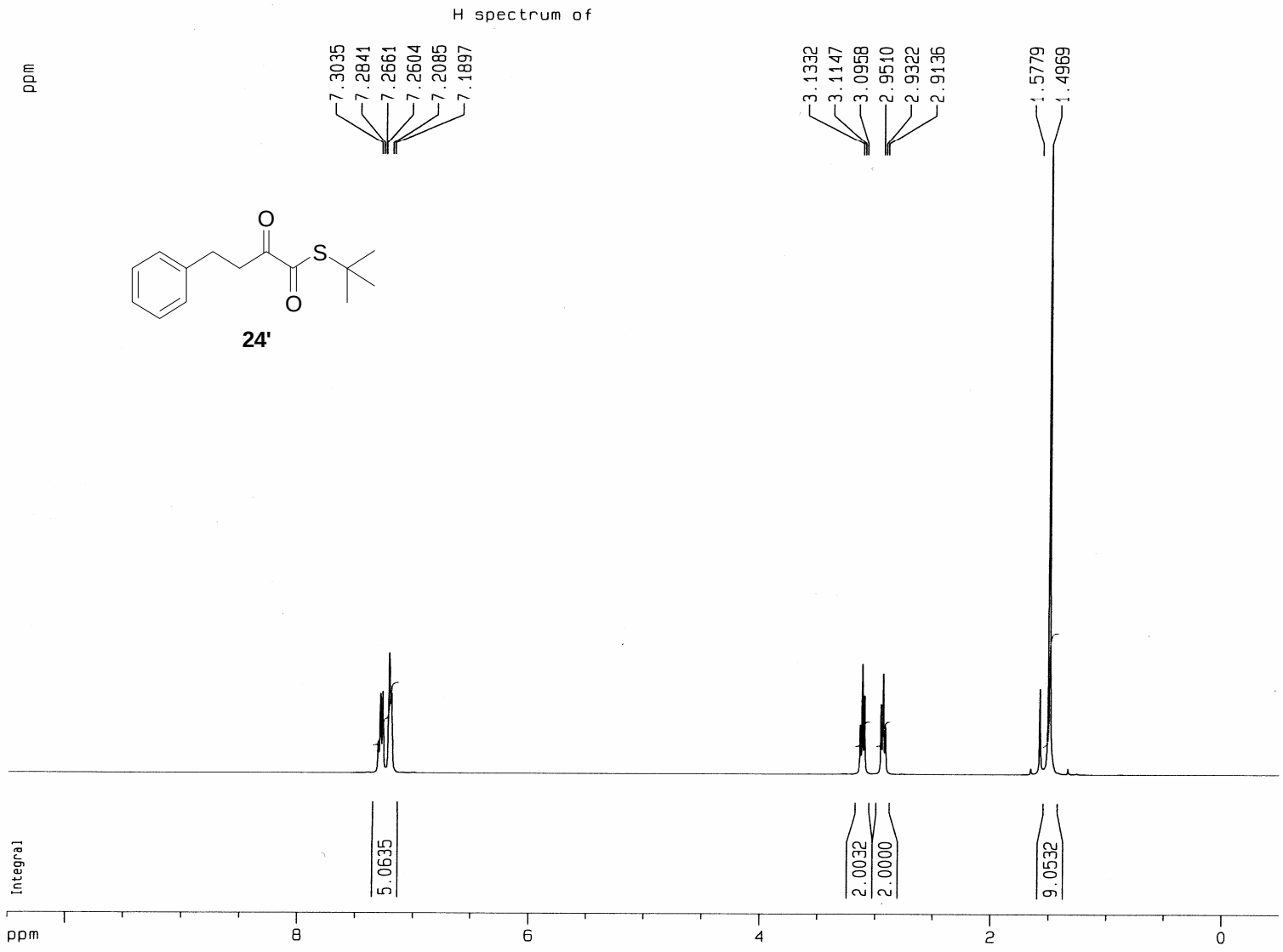
```
Current Data Parameters
NAME        sam-Cinam-HT
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_          20060426
Time              18.38
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                16384
SOLVENT           CDCl3
NS                    4
DS                    0
SWH            5995.204 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG               456.1
DW               83.400 usec
DE                6.50 usec
TE               300.0 K
D1            1.50000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.10 usec
PL1               3.00 dB
SFO1        400.1326008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300095 MHz
WDW                  EM
SSB                   0
LB                 0.10 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                20.00 cm
F1P              10.500 ppm
F1             4201.37 Hz
F2P              -0.500 ppm
F2             -200.06 Hz
PPMCM          0.55000 ppm/cm
HZCM         220.07150 Hz/cm
```

C13 spectrum of



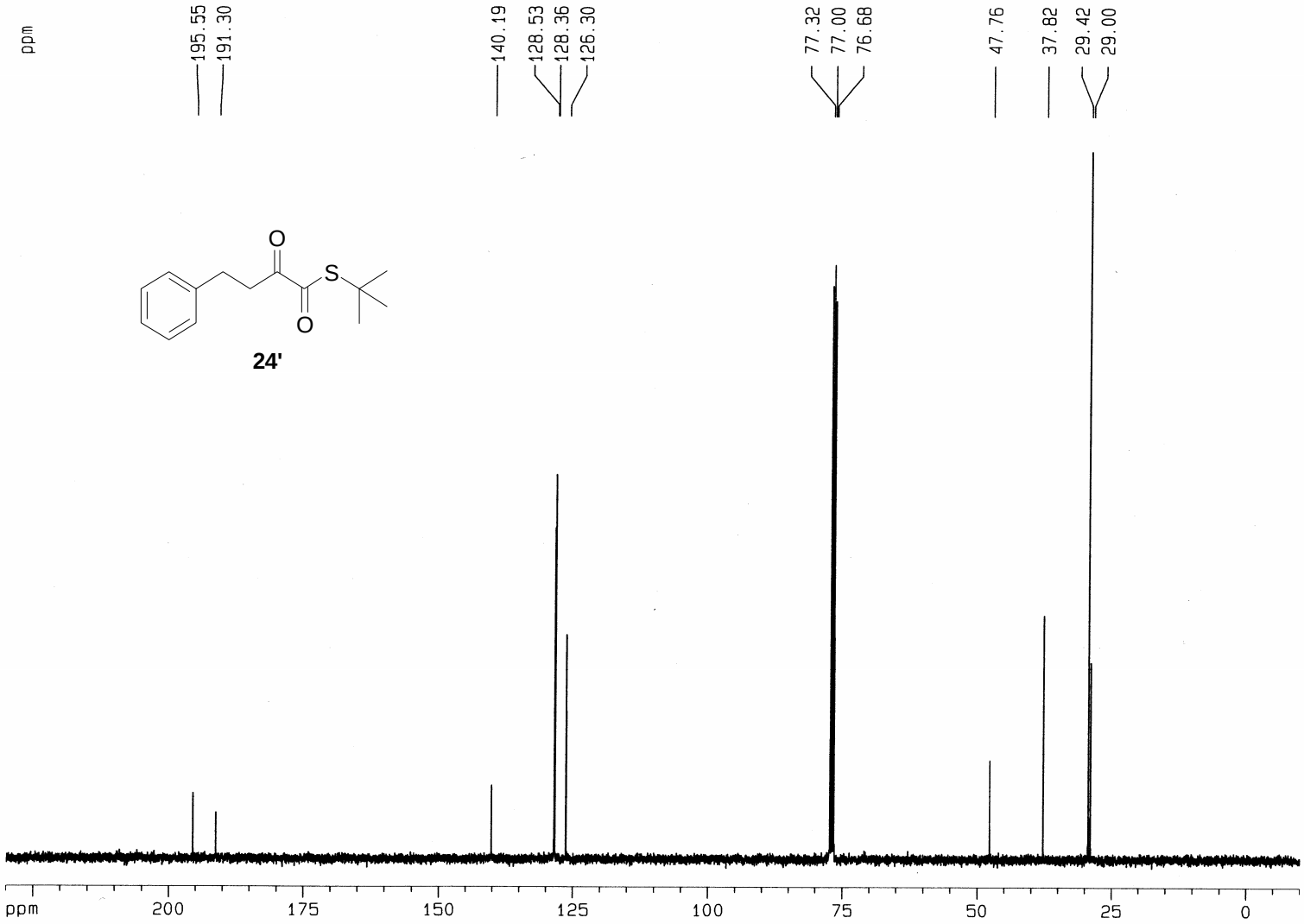
23'

```
Current Data Parameters
NAME        sam-Cinam-HT
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20060426
Time               19 16
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1446
DS                    0
SWH            25125.629 Hz
FIDRES          0.383387 Hz
AQ             1.3042164 sec
RG                 8192
DW               19.900 usec
DE                6.50 usec
TE               300.0 K
D1             1.20000005 sec
d11            0.03000000 sec
d12            0.00002000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.80 usec
PL1                 7.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12              21.83 dB
PL13              24.80 dB
SFO2        400.1319000 MHz

F2 - Processing parameters
SI                32768
SF          100.6127706 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 12.50 cm
F1P               210.000 ppm
F1             21126.66 Hz
F2P               -10.000 ppm
F2             -1006.13 Hz
PPMCM             11.00000 ppm/cm
HZCM           1106.74048 Hz/cm
```



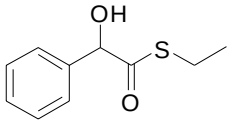

```
Current Data Parameters
NAME                Alp-ket
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_             20060930
Time                 12.29
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG               zg30
TD                    16384
SOLVENT               CDCl3
NS                       32
DS                        0
SWH               5995.204 Hz
FIDRES            0.365918 Hz
AQ               1.3664756 sec
RG                   203.2
DW                  83.400 usec
DE                    6.50 usec
TE                   298.1 K
D1             1.50000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   10.30 usec
PL1                   2.00 dB
SFO1           400.1326008 MHz

F2 - Processing parameters
SI                    16384
SF             400.1300099 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.00

1D NMR plot parameters
CX                    20.00 cm
CY                    20.00 cm
F1P                  10.500 ppm
F1                 4201.37 Hz
F2P                  -0.500 ppm
F2                  -200.06 Hz
PPMCM              0.55000 ppm/cm
HZCM             220.07150 Hz/cm
```

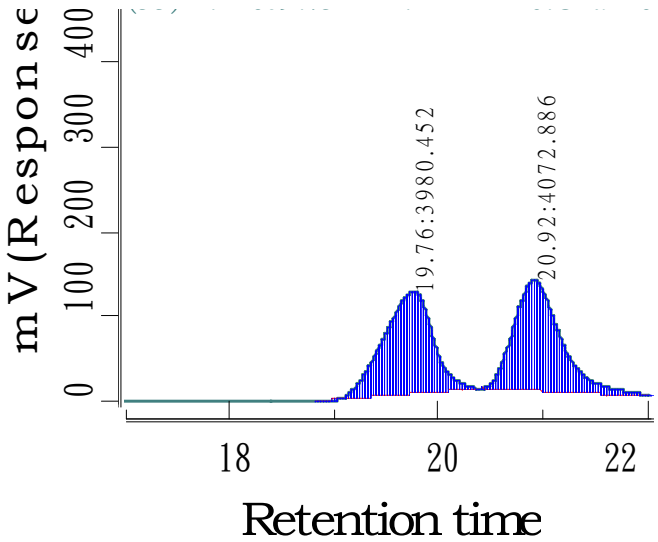
C13 spectrum of




```
Current Data Parameters
NAME                Alp-ket
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_             20060930
Time                 12.32
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    545
DS                      0
SWH             25125.629 Hz
FIDRES           0.383387 Hz
AQ               1.3042164 sec
RG                   8192
DW                  19.900 usec
DE                   6.50 usec
TE                  298.2 K
D1             1.20000005 sec
d11            0.03000000 sec
DELTA          1.10000002 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                  10.00 usec
PL1                  3.00 dB
SFO1          100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               90.00 usec
PL2                  2.00 dB
PL12                20.80 dB
PL13                23.80 dB
SFO2          400.1319000 MHz

F2 - Processing parameters
SI                   32768
SF            100.6127721 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40

1D NMR plot parameters
CX                   20.00 cm
CY                   12.50 cm
F1P                 230.000 ppm
F1                 23140.94 Hz
F2P                 -10.000 ppm
F2                 -1006.13 Hz
PPMCM              12.00000 ppm/cm
HZCM            1207.35315 Hz/cm
```

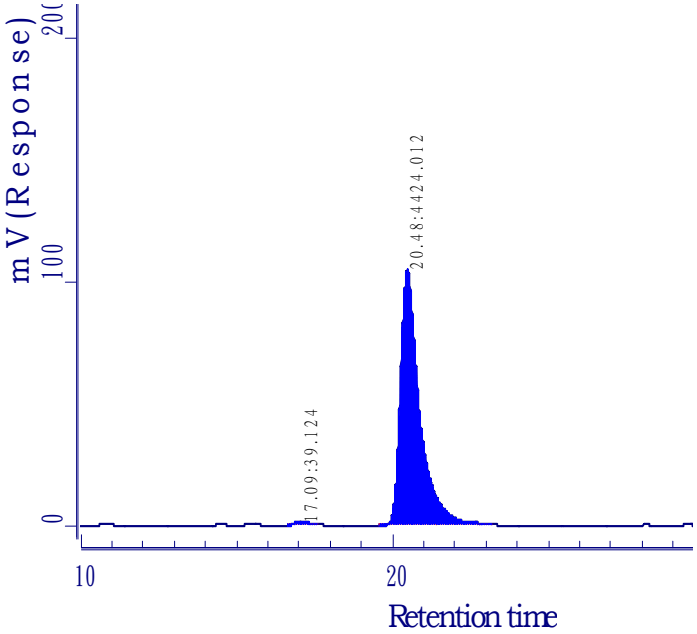
Racemic (97/3, AD-H) (**8a**)





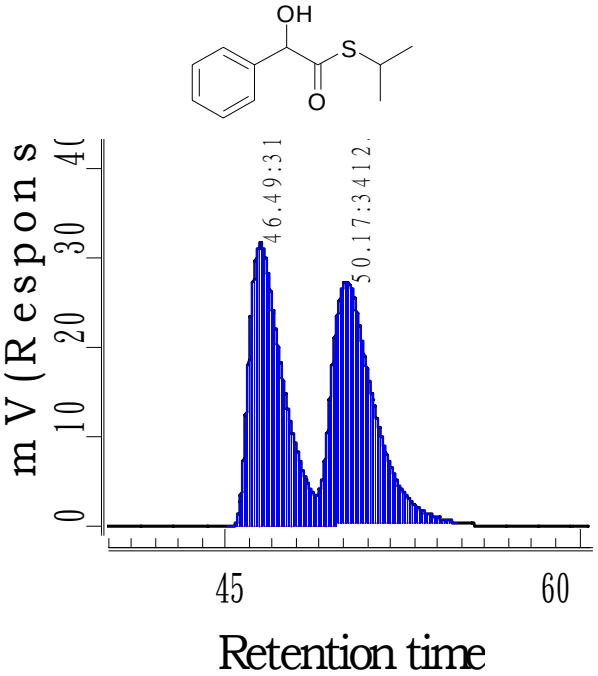
#	成分峰名稱	滯留時間	面積	百分比	濃度
0		19.764	3980.45	49.43	0.00
1		20.917	4072.89	50.57	0.00

Resolved



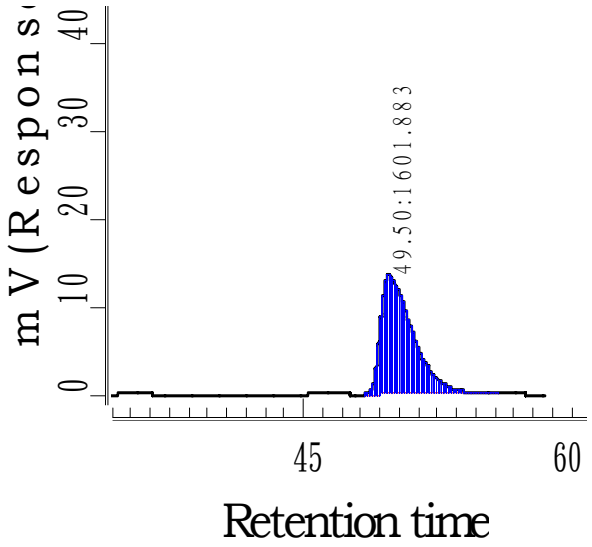
#	成分峰名稱	滯留時間	Area	百分比	濃度
0		17.085	39.12	0.88	0.00
1		20.482	4424.01	99.12	0.00

Racemic (99/1, AD-H) (**8b**)



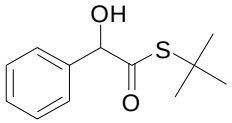
#	成分峰名稱	滯留時間	Area	百分比	濃度
0		46.490	3179.21	48.23	0.00
1		50.167	3412.38	51.77	0.00

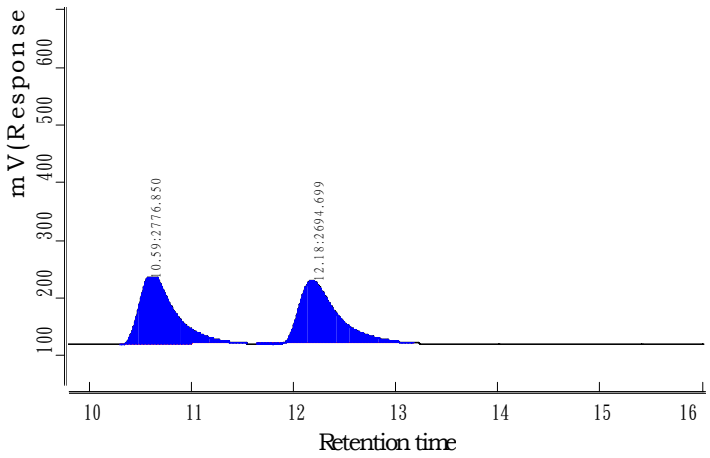
Resolved



#	成分峰名稱	滯留時間	Area	百分比	濃度
0		49.499	1601.88	100.00	0.00

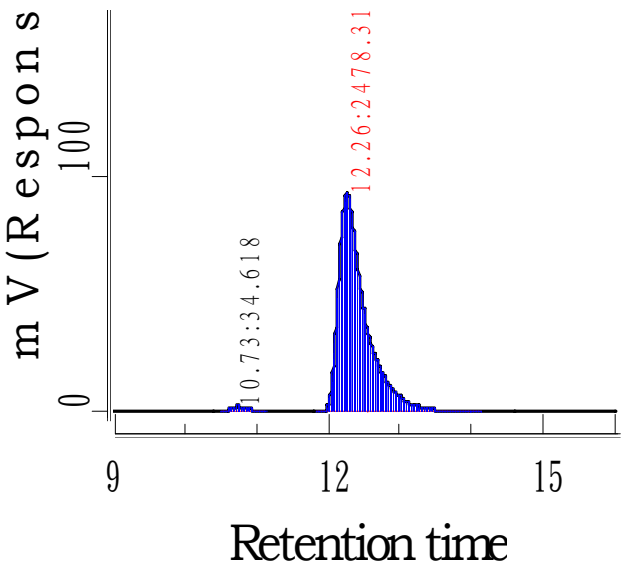
Racemic (94/6, AD-H) (**8c**)





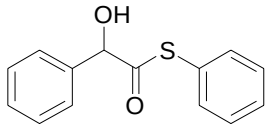
#	成分峰名稱	滯留時間	Area	百分比	濃度
0		10.588	2776.85	50.75	0.00
1		12.184	2694.70	49.25	0.00

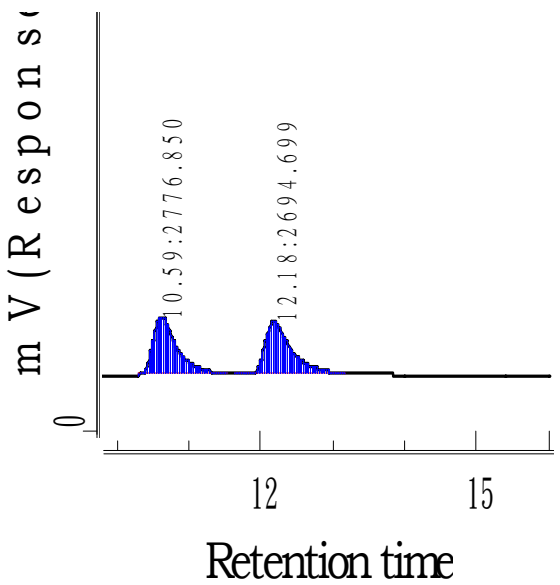
Resolved



#	成分峰名稱	滯留時間	Area	百分比	濃度
0		10.729	34.62	1.38	0.00
1		12.262	2478.32	98.62	0.00

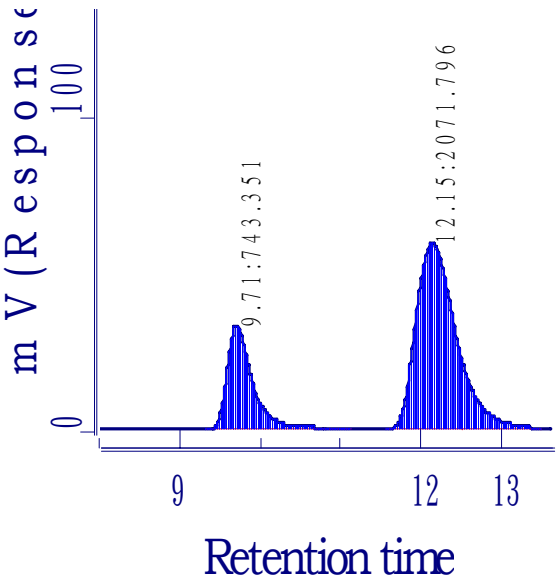
Racemic (94/6, AD-H) (**8e**)





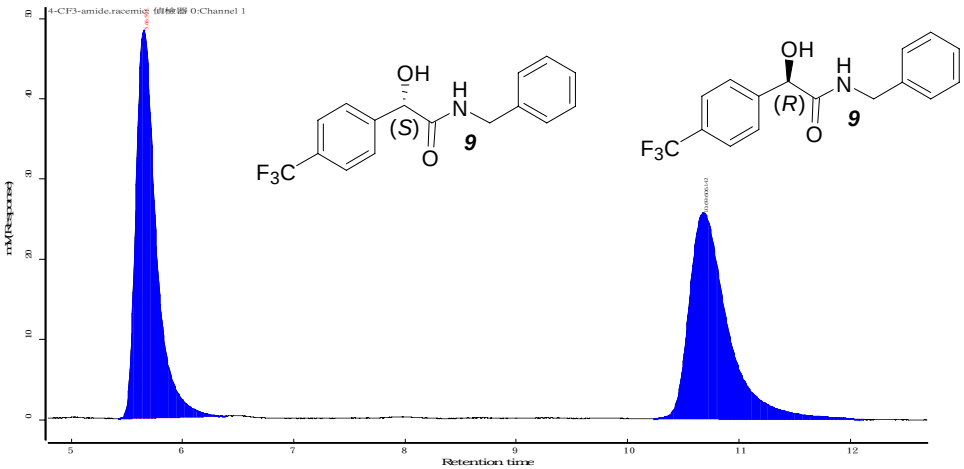
#	成分峰名稱	滯留時間	Area	百分比	濃度
0		10.588	2776.85	50.75	0.00
1		12.184	2694.70	49.25	0.00

Resolved



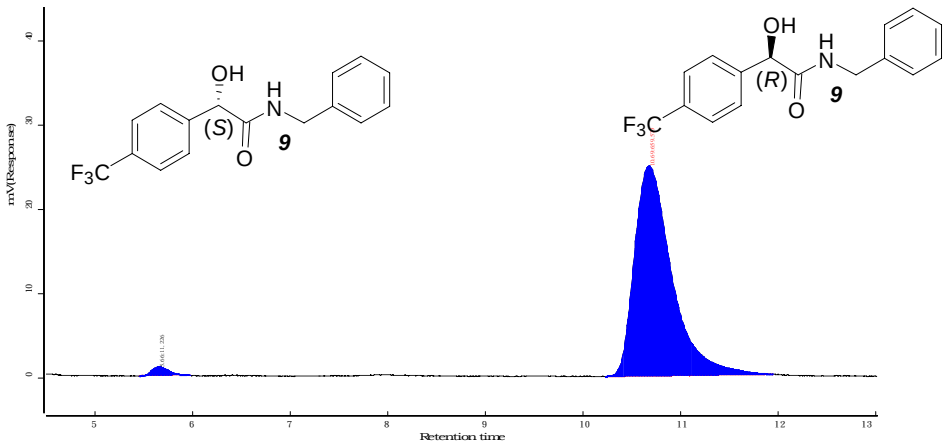
#	成分峰名稱	滯留時間	Area	百分比	濃度
0		9.709	743.35	26.41	0.00
1		12.149	2071.80	73.59	0.00

Racemic (88/12, AD-H) (**9**)



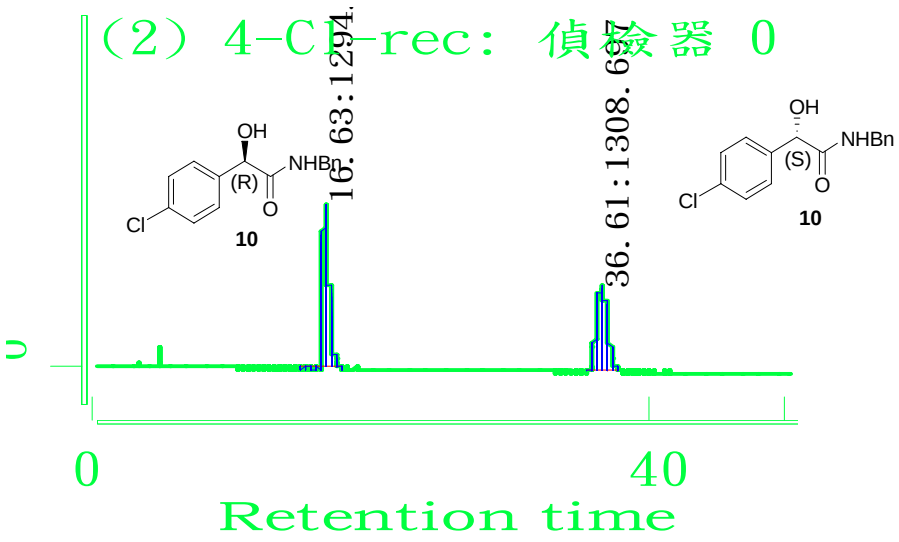
#	成分峰名稱	滯留時間	面積	百分比	濃度
0		5.659	595.19	49.54	0.00
1		10.686	606.14	50.46	0.00

Resolved



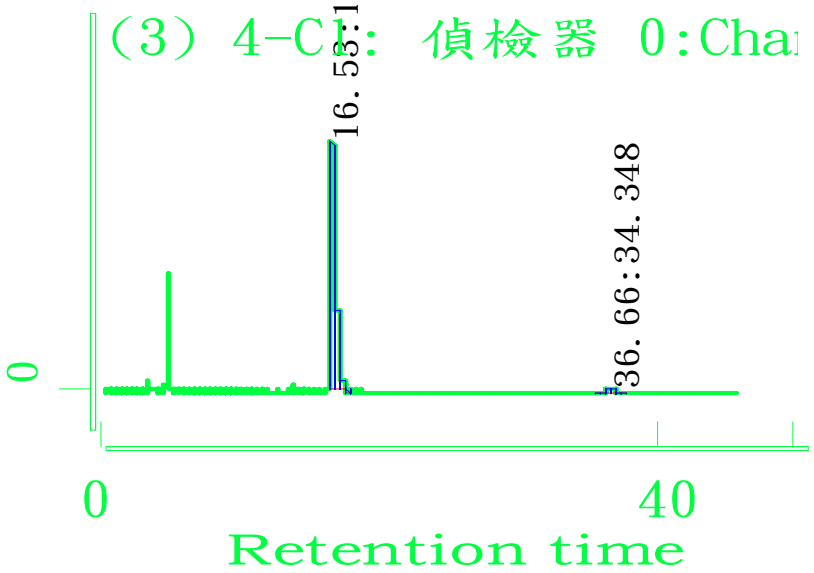
#	成分峰名稱	滯留時間	面積	百分比	濃度
0		5.659	11.23	1.67	0.00
1		10.687	659.58	98.33	0.00

Racemic **10**: Chiralcel AD-H, ^{i}PrOH/Hexane=8/92



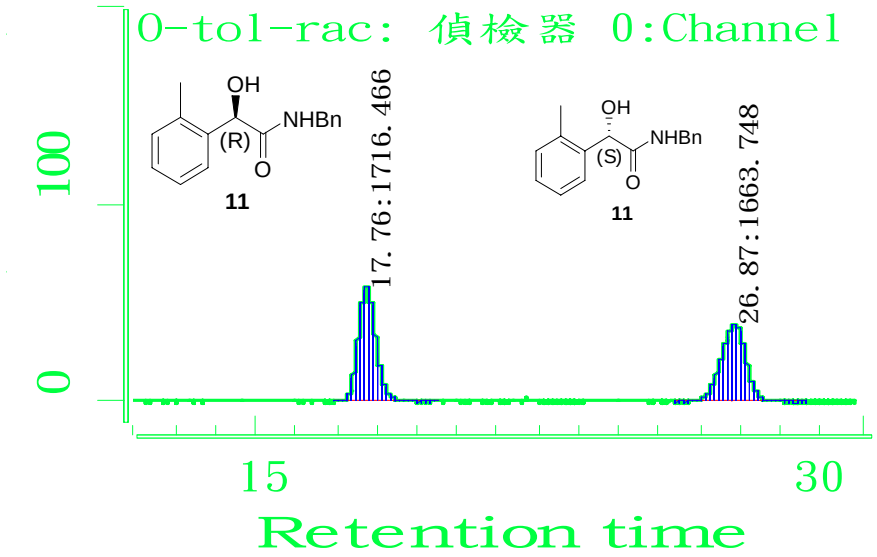
滯留時間	面積	百分比	濃度
16.634	1294.52	49.73	0.00
36.607	1308.70	50.27	0.00

Resolved



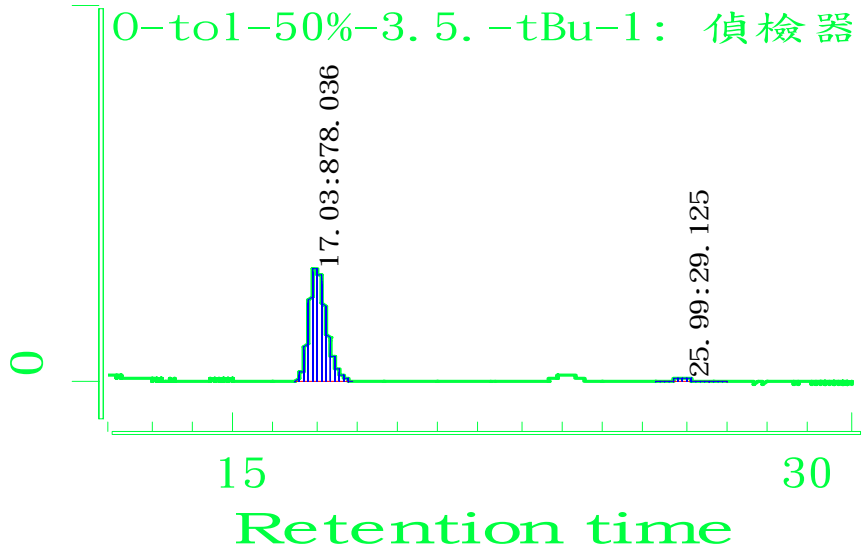
滯留時間	面積	百分比	濃度
16.529	1921.12	98.24	0.00
36.658	34.35	1.76	0.00

Racemic **11**: Chiralcel AD-H, ^{i}PrOH/Hexane=8/92



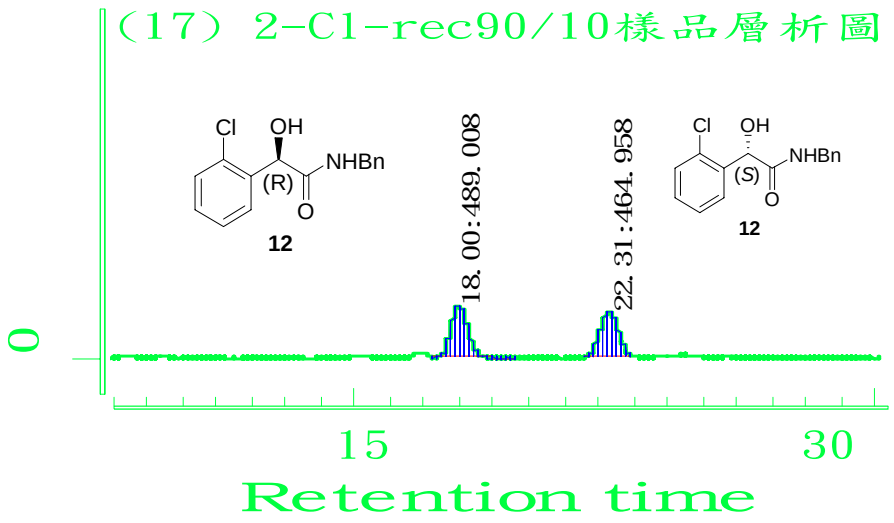
滯留時間	面積	百分比	濃度
17.764	1716.47	50.78	0.00
26.867	1663.75	49.22	0.00

Resolved



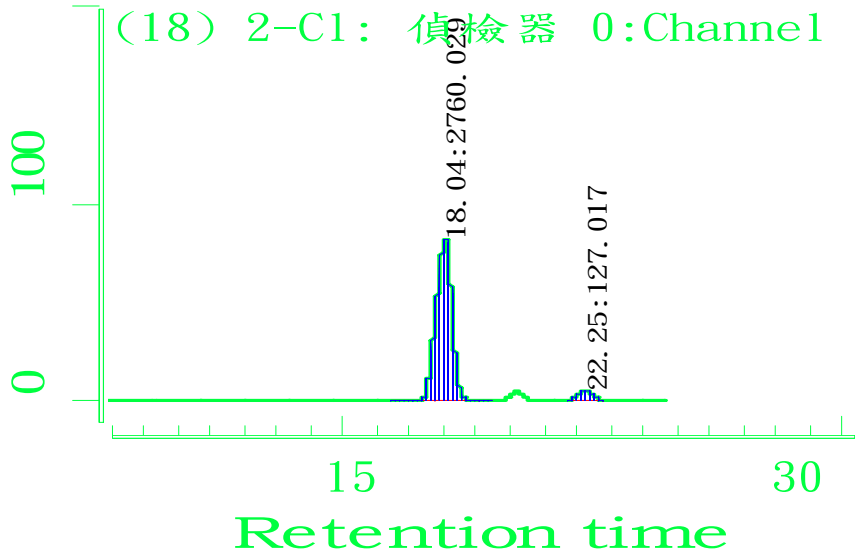
滯留時間	面積	百分比	濃度
17.026	878.04	96.79	0.00
25.990	29.12	3.21	0.00

Racemic **12**: Chiralcel AD-H, ^{i}PrOH/Hexane=10/90



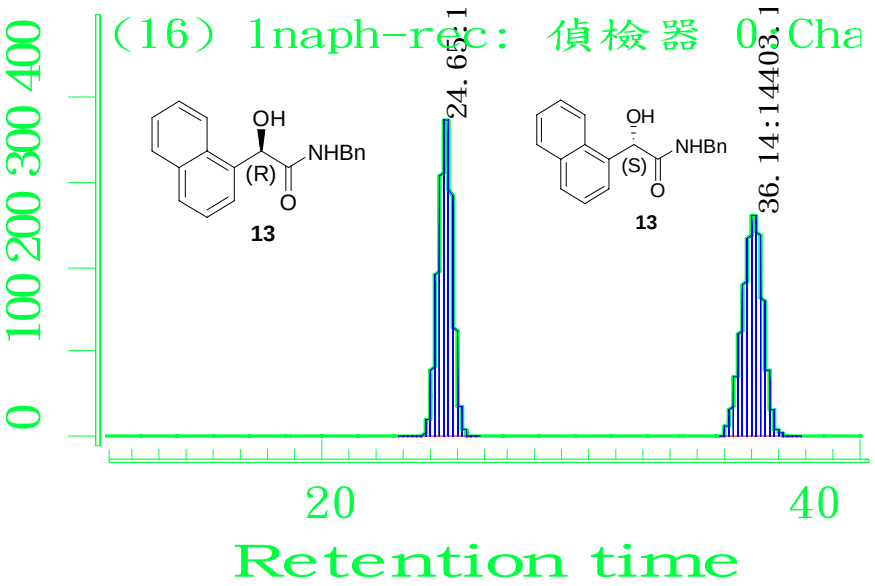
滯留時間	面積	百分比	濃度
17.998	489.01	51.26	0.00
22.314	464.96	48.74	0.00

Resolved



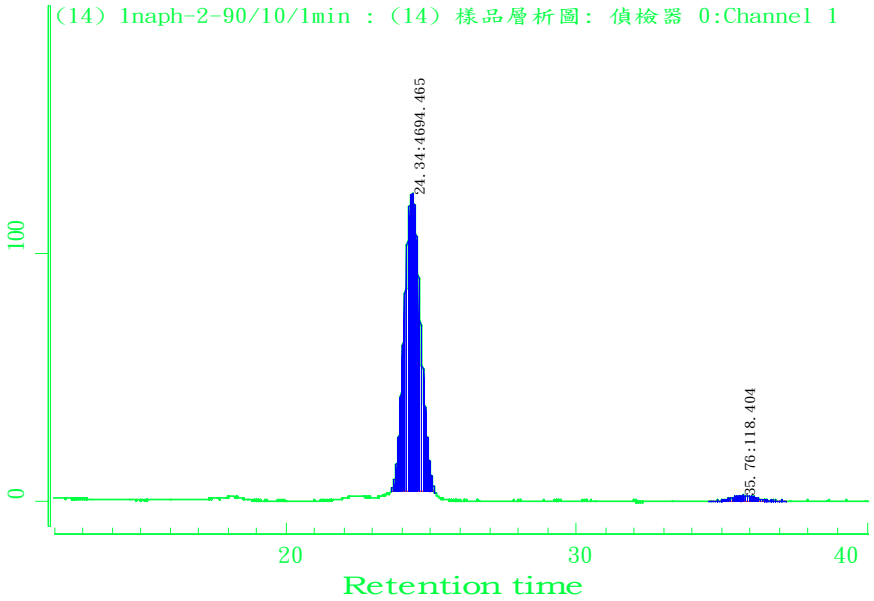
滯留時間	面積	百分比	濃度
18.041	2760.03	95.60	0.00
22.246	127.02	4.40	0.00

Racemic **13**: Chiralcel AD-H, ^{i}PrOH/Hexane=10/90



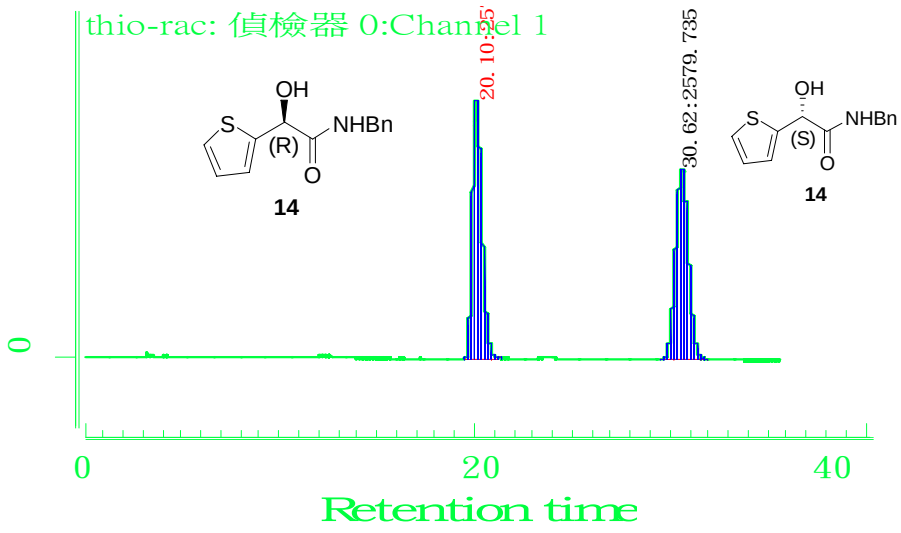
滯留時間	面積	百分比	濃度
24.649	14550.98	50.26	0.00
36.143	14403.16	49.74	0.00

Resolved



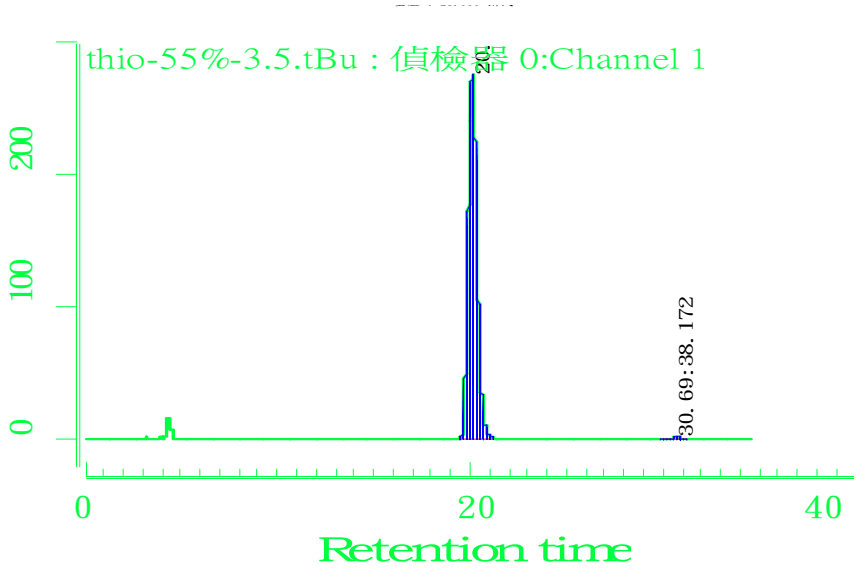
滯留時間	面積	百分比	濃度
24.343	4694.46	97.54	0.00
35.755	118.40	2.46	0.00

Racemic **14**: Chiralcel AD-H, ^{i}PrOH/Hexane = 8/92



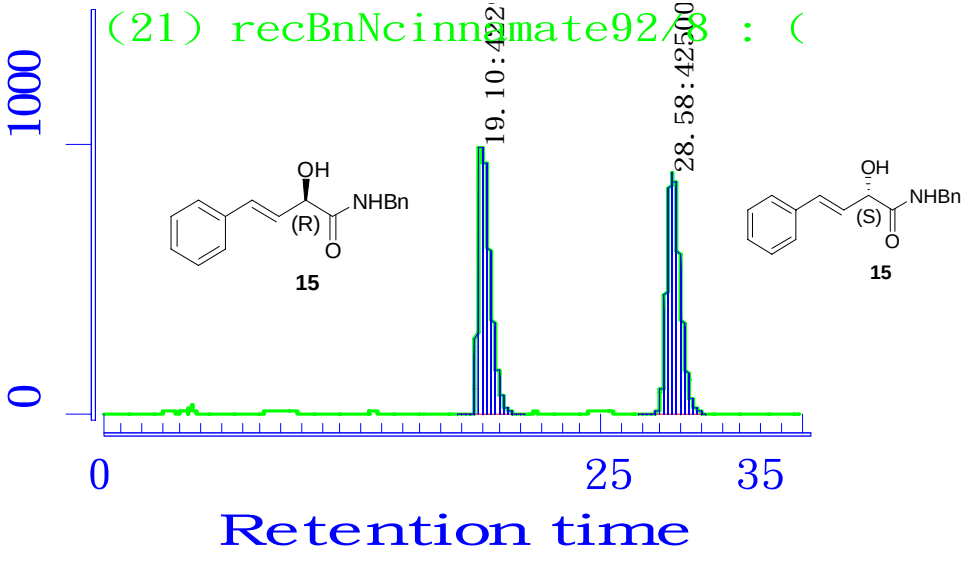
滯留時間	面積	百分比	濃度
20.105	2579.85	50.00	0.00
30.622	2579.74	50.00	0.00

Resolved



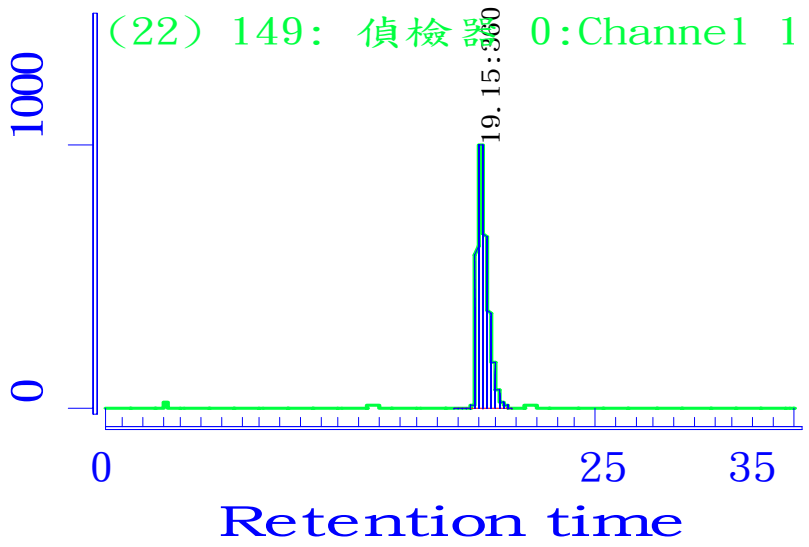
滯留時間	面積	百分比	濃度
20.131	9162.53	99.59	0.00
30.685	38.17	0.41	0.00

Racemic **15**: Chiralcel AD-H, ^{i}PrOH/Hexane = 8/92



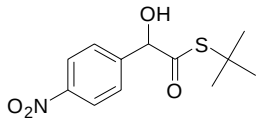
滯留時間	面積	百分比	濃度
19.099	42296.42	49.88	0.00
28.577	42500.96	50.12	0.00

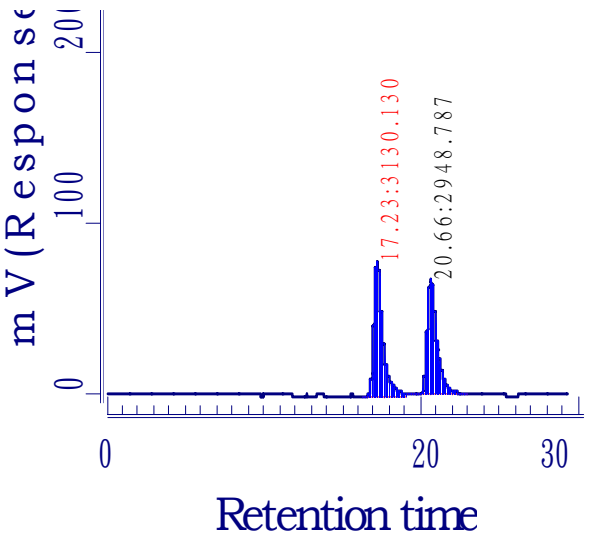
Resolved



滯留時間	面積	百分比	濃度
19.150	36051.83	100.00	0.00

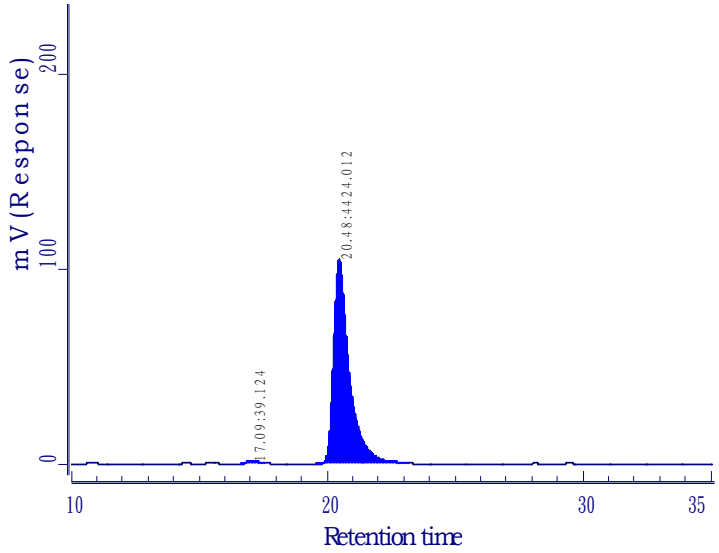
Racemic (94/6, AD-H) (**16**)





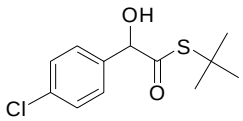
#	成分峰名稱	滯留時間	Area	百分比	濃度
0		17.233	3130.13	51.49	0.00
1		20.657	2948.79	48.51	0.00

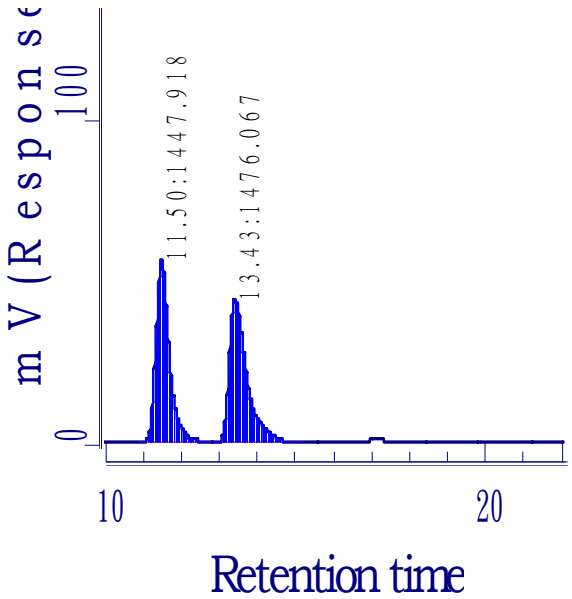
Resolved



#	成分峰名稱	滯留時間	Area	百分比	濃度
0		17.085	39.12	0.88	0.00
1		20.482	4424.01	99.12	0.00

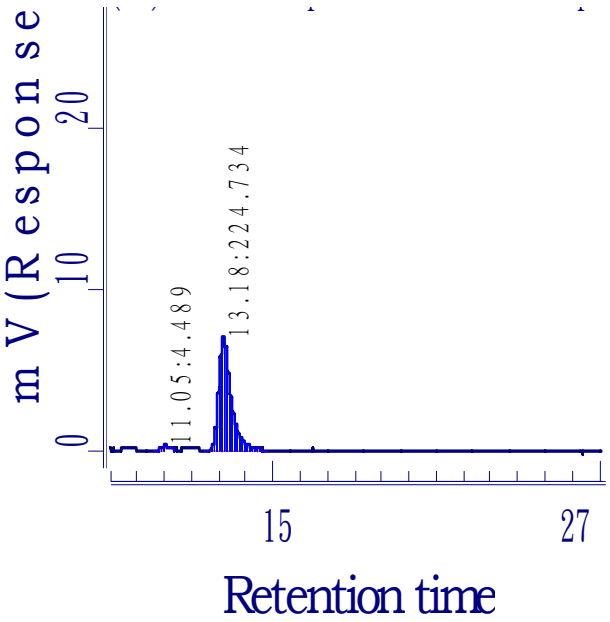
Racemic (94/6, AD-H) (**17**)





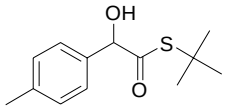
#	成分峰名稱	滯留時間	Area	百分比	濃度
0		11.495	1447.92	49.52	0.00
1		13.429	1476.07	50.48	0.00

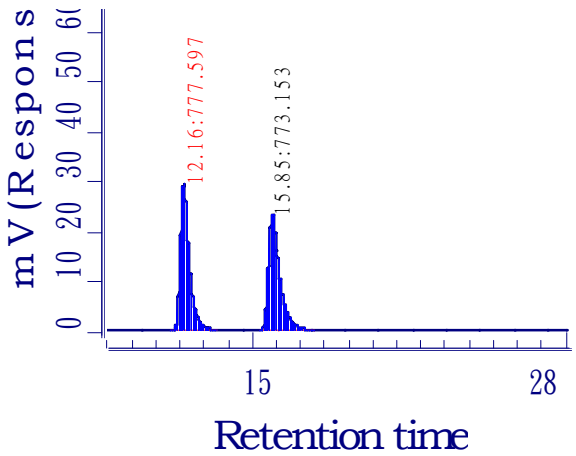
Resolved



#	成分峰名稱	滯留時間	Area	百分比	濃度
0		11.051	4.49	1.96	0.00
1		13.179	224.73	98.04	0.00

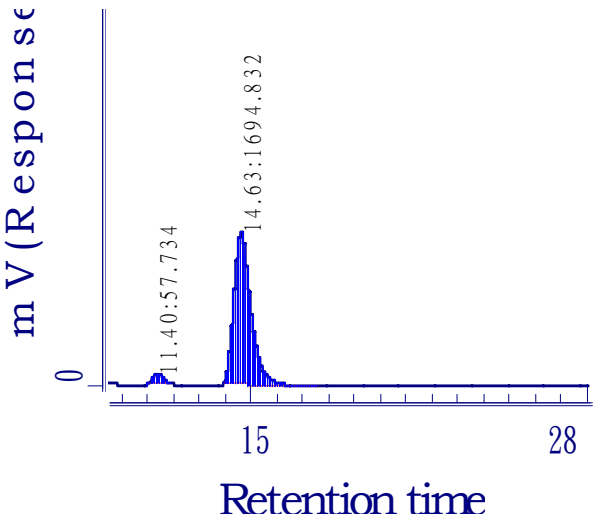
Racemic (94/6, AD-H) (**18**)





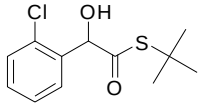
#	成分峰名稱	滯留時間	Area	百分比	濃度
0		12.156	777.60	50.14	0.00
1		15.847	773.15	49.86	0.00

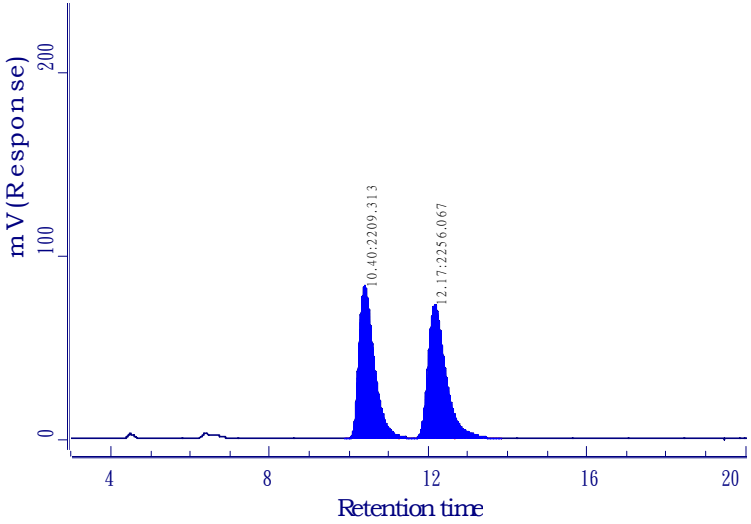
Resolved



#	成分峰名稱	滯留時間	Area	百分比	濃度
0		11.401	57.73	3.29	0.00
1		14.628	1694.83	96.71	0.00

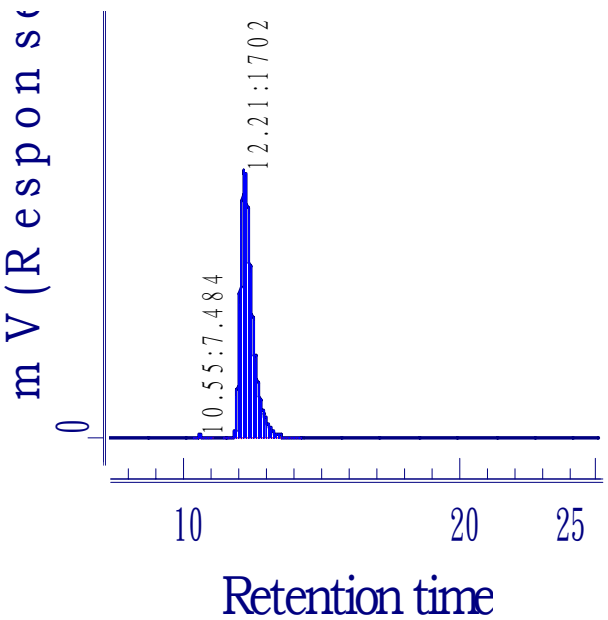
Racemic (94/6, AD-H) (**19**)





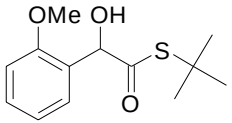
#	成分峰名稱	滯留時間	Area	百分比	濃度
0		10.398	2209.31	49.48	0.00
1		12.170	2256.07	50.52	0.00

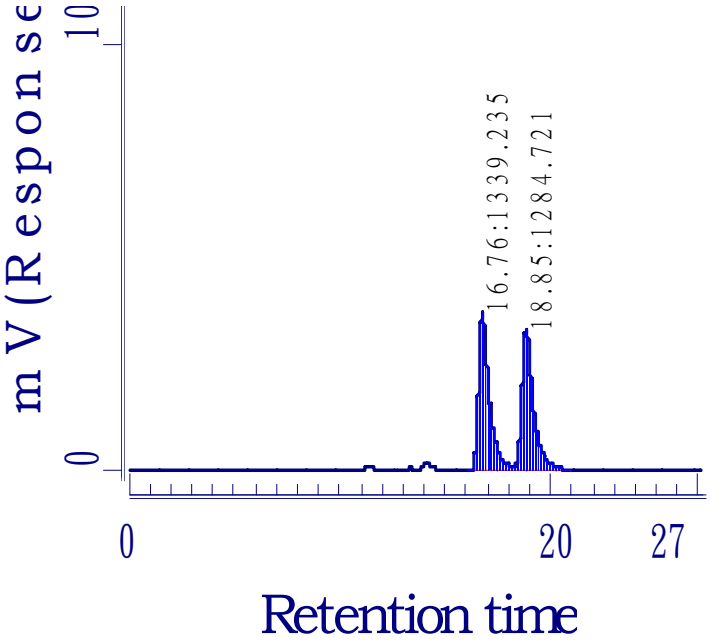
Resolved



#	成分峰名稱	滯留時間	Area	百分比	濃度
0		10.551	7.48	0.44	0.00
1		12.210	1702.57	99.56	0.00

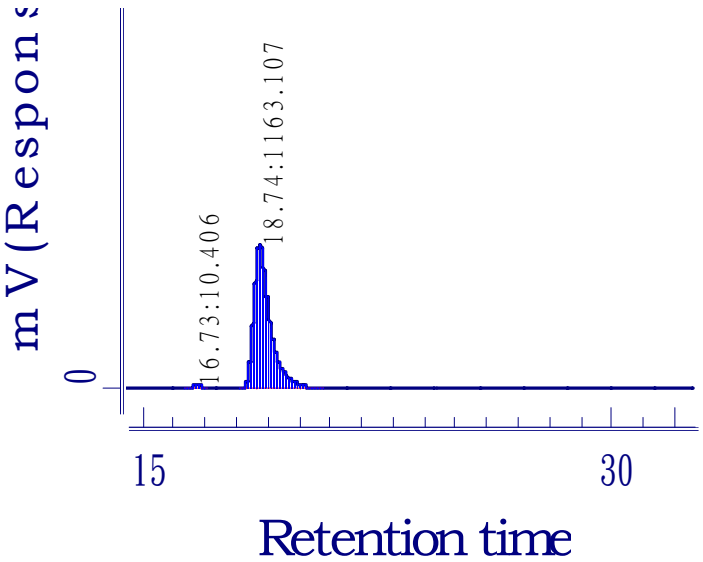
Racemic (94/6, AD-H) (**20**)





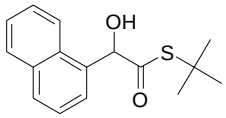
#	成分峰名稱	滯留時間	Area	百分比	濃度
0		16.759	1339.24	51.04	0.00
1		18.847	1284.72	48.96	0.00

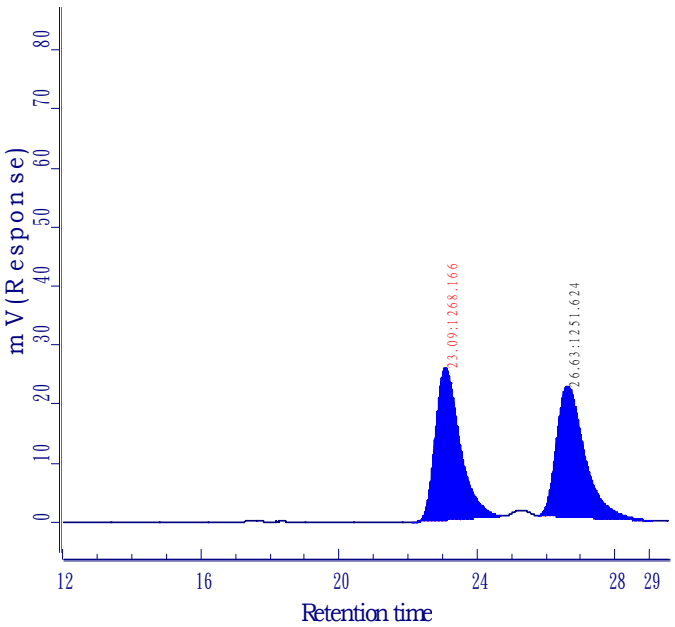
Resolved



#	成分峰名稱	滯留時間	Area	百分比	濃度
0		16.726	10.41	0.89	0.00
1		18.744	1163.11	99.11	0.00

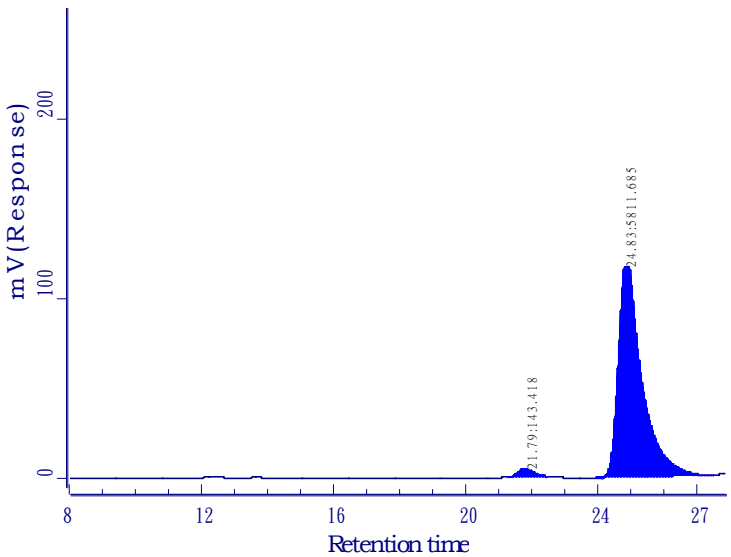
Racemic (96/4, AD-H) (**21**)





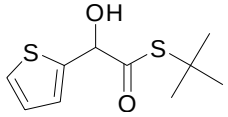
#	成分峰名稱	滯留時間	Area	百分比	濃度
0		23.090	1268.17	50.33	0.00
1		26.634	1251.62	49.67	0.00

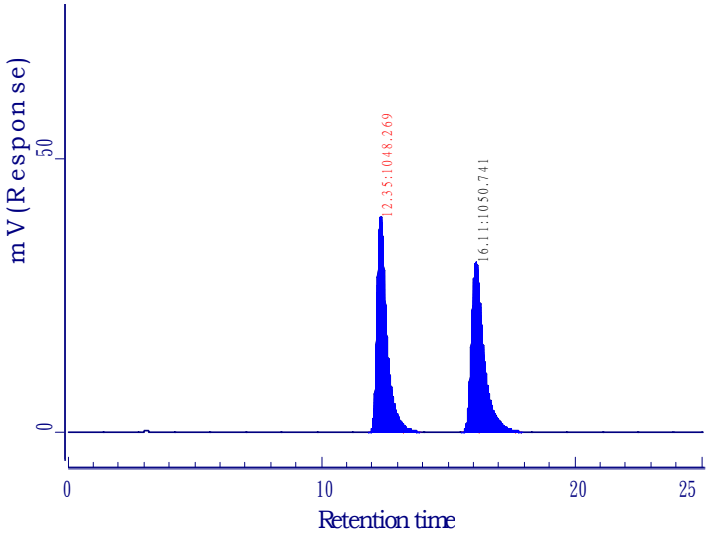
Resolved



#	成分峰名稱	滯留時間	Area	百分比	濃度
0		21.794	143.42	2.41	0.00
1		24.831	5811.68	97.59	0.00

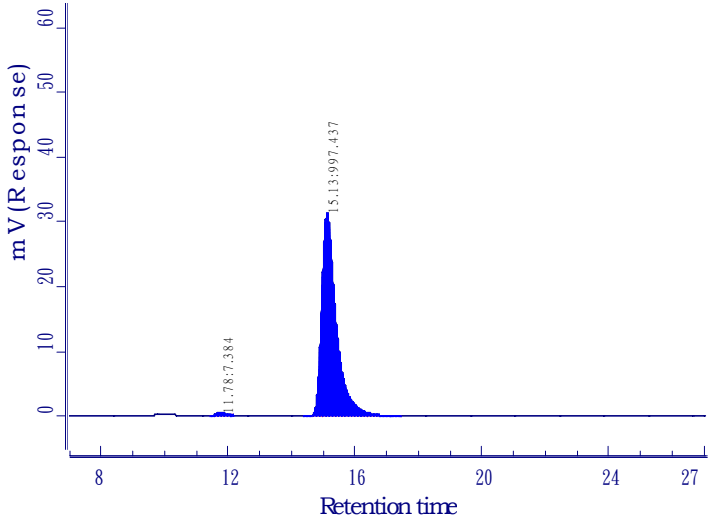
Racemic (94/6, AD-H) (**22**)





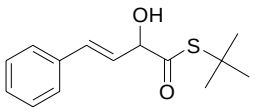
#	成分峰名稱	滯留時間	Area	百分比	濃度
0		12.353	1048.27	49.94	0.00
1		16.115	1050.74	50.06	0.00

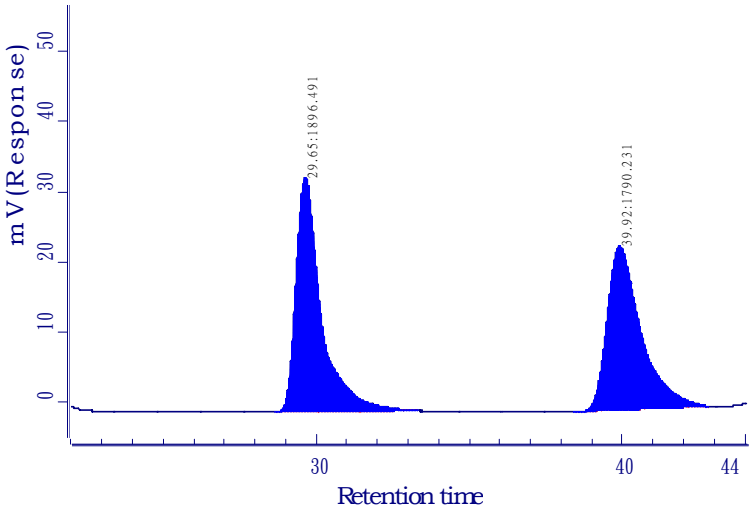
Resolved



#	成分峰名稱	滯留時間	Area	百分比	濃度
0		11.784	7.38	0.73	0.00
1		15.130	997.44	99.27	0.00

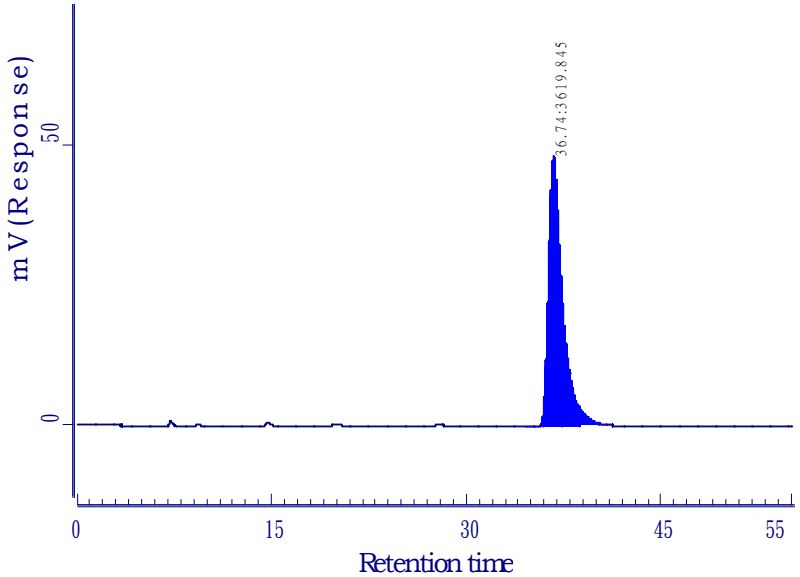
Racemic (98/2, AD-H) (**23**)





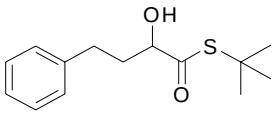
#	成分峰名稱	滯留時間	Area	百分比	濃度
0		29.655	1896.49	51.44	0.00
1		39.920	1790.23	48.56	0.00

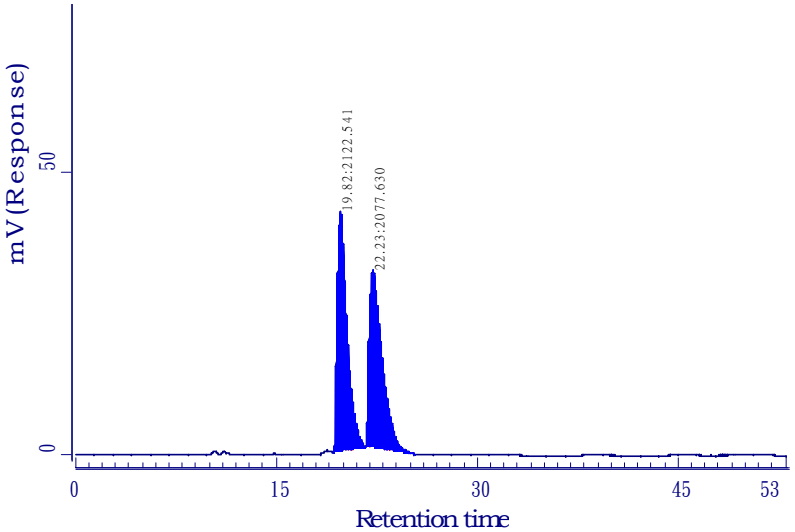
Resolved



#	成分峰名稱	滯留時間	Area	百分比	濃度
0		36.744	3619.84	100.00	0.00

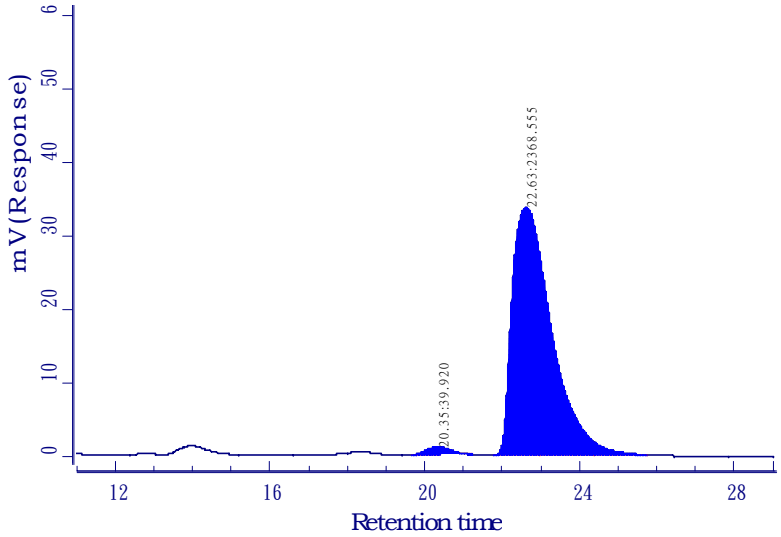
Racemic (98/2, AD-H) (**24**)





#	成分峰名稱	滯留時間	Area	百分比	濃度
0		19.820	2122.54	50.53	0.00
1		22.225	2077.63	49.47	0.00

Resolved



#	成分峰名稱	滯留時間	Area	百分比	濃度
0		20.348	39.92	1.66	0.00
1		22.626	2368.55	98.34	0.00